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INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

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(51) International Patent Classification 6 : C07K	A2	(11) International Publication Numbe	: WO 99/60014		
		(43) International Publication Date:	25 November 1999 (25.11.99)		

(21) International Application Number:

PCT/US99/06899

(22) International Filing Date:

30 March 1999 (30.03.99)

(30) Priority Data:

60/079,956 30 March 1998 60/113,146 16 December 19

30 March 1998 (30.03.98) US 16 December 1998 (16.12.98) US

(71) Applicant: THE REGENTS OF THE UNIVERSITY OF CALIFORNIA [US/US]; 12th floor, 1111 Franklin Street, Oakland, CA 94607-5200 (US).

(72) Inventors: BAXTER, John, D.; 131 San Pablo Avenue, San Francisco, CA 94127 (US). DARIMONT, Beatrice; 1441 Tenth Avenue, San Francisco, CA 94122 (US). FENG, Weijun; 105 Johnstone Drive, San Francisco, CA 94131 (US). FLETTERICK, Robert; 15 Christopher Avenue, San Francisco, CA 94131 (US). KUSHNER, Peter, J.; 1362 6th Avenue, San Francisco, CA 94122 (US). WAGNER, Richard, L.; 1701 Waller Street, San Francisco, CA 94117 (US). WEST, Brian, L.; 142 Anderson Street, San Francisco, CA 94110 (US). YAMAMOTO, Keith, R.; 332 Douglass Street, San Francisco, CA 94114 (US).

(74) Agents: BRADBURNE, James, A.; Cooley Godward LLP, 3000 El Camino Real, Five Palo Alto Square, Palo Alto, CA 94306-2155 (US) et al.

(81) Designated States: AU, CA, JP, KR, European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).

Published

Without international search report and to be republished upon receipt of that report.

(54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(57) Abstract

The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

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METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

ACKNOWLEDGEMENTS

This invention was supported in part by grants from the National Institutes of Health: Grant Nos. DK 51083, DK 51281, and P41-RR01081 and from the Army of the United States: Grant No. AIBS#562. The U.S. Government may have rights in this invention.

INTRODUCTION

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Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

Although overall sequence conservation between nuclear receptors varies between different families of receptors, sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to modulate transcription of DNA, although they may have transcription-independent actions. Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear receptors on transcription. For example, nuclear receptors can stimulate transcription in response to hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al., Curr. Opin. Cell Biol. (1997) 9:222-32); and Horwitz et al., Mol. Endocrinol. (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain, called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253; VDR: Jurutka et al., J. *Biol. Chem.* (1997) 227:14592-14599. Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-1839). While these studies support the physiological relevance of the observed interaction, the structural and functional nature of the site to which coactivators bind has not been defined.

The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism, hypercholesterolemia, obesity and other conditions. However, limited treatments are available and current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors are desired for drug development, the structural and functional basis of such sites, including the coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator proteins. This would provide a major new target for iterative drug design, synthesis, and selection. It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target the coactivator binding site of nuclear receptors and administer them to organisms to modulate physiological processes regulated by nuclear receptors.

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5 Relevant Literature

Wagner et al., (Nature (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., supra; O'Donnell et al., Mol. Endocrinol. (1991) 5:94-99; Whitfield et al., Mol. Endocrinol. (1995) 9:1166-79; Saatcioglu et al., Mol. Cell Biol. (1997) 17:4687-95; Collingwood et al., supra; Kamei et al., Cell (1996) 85:403-14). Hong et al. (Proc. Natl. Acad. Sci. USA (1996) 93(10):498-49452) and Hong et al. (Mol. Cell. Biol. (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (Nature (1997) 387:677-84), Le Douarin et al., (EMBO J (1996) 15:6701-6715) and Heery et al. (Nature (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

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SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by

binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be in vitro or in vivo. The method comprises administering, in vitro or in vivo, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

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5 binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the specific effects of mutations on hTRβ1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T₃ dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant. GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

Figure 2 shows that overexpression of full-length GRIP1 rescues loss of transcriptional activation by hTRβ1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in Figure 1. The WT or different representative hTRβ1 mutants are indicated.

Figure 3 shows specific hER α surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E₂ activation, expressed as the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [35 S]-labeled hER α WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

5 Figure 4 shows a plot of the fold E2 activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for Figure 3. The WT or different hERa mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

10 Figure 5 shows a CPK model of the $TR\alpha$ -LBD, indicating the LBD surface locations of mutations made in the full-length hTR\$1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1a binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues, respectively. The main chain structures of the $TR\alpha$ - and $TR\beta$ -LBDs are the same (data not shown). 15

Figure 6 shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

Figure 7 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, 20 and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TRβ LBD. Single letter designations are used for the amino acids.

Figure 8 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

25 Figure 9 shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

Figure 10 shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of NR-box-TRβ LBD interactions.

Figure 11 shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TRβ LBD.

Figure 12 shows the contents of the asymmetric unit of the crystallized hTRß LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in both bound peptides.

Figure 13 shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR β LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of α -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR β LBD, and the neighboring monomer, are omitted for clarity.

Figure 14 shows interface between the GRIP1 NR-box 2 peptide and the hTR\$ LBD. Side chains of residues of the hTR\$ LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID NO: 2) ILxxLL motif shown explicitly.

Figure 15 shows residues in the hTRB LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTRB LBD.

Figure 16 shows molecular surface of the hTR LBD. The side chains of the leucines resides fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

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Figure 17 shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucince residues fit into pockets of the coactivator binding site of the hTRB LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

Figure 18 shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

Figure 19 shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

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DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284. Lys288. Ile302, Lys306. Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

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for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

Compounds of particular interest fit spacially and preferentially into the coactivator binding By "fits spacially and preferentially" is intended that a compound possesses a threedimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single

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gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α , β) or three (RAR, RXR, and PPAR: α , β , γ) genes or have alternate RNA splicing.

The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in Figure 19). As described in the Examples, the cocrystal of the hTRB LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide. Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO: 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule databases include any virtual or physical database, such as electronic and physical compound library databases. and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR), using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

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molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, *J. Med. Chem.* (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., *Proteins: Structure, Function and Genetics*, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., *Proteins: Structure, Function and Genetics* (1990) 8:195-202; available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, *J. Mol. Biol.* (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

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Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, for example, Farmer, "*Drug Design*," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity, such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

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preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

As an example, in vitro binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein and in Shibata et al. (Recent Prog. Horm. Res. 52:141-164 (1997)); Tagami et al. (Mol. Cell Biol. (1997) 17(5):2642-2648); Zhu et al. (J. Biol. Chem. (1997) 272(14):9048-9054); Lin et al. (Mol. Cell Biol. (1997) 17(10):6131-6138); Kakizawa et al. (J. Biol. Chem. (1997) 272(38):23799-23804); and Chang et al. (Proc. Natl. Acad. Sci. USA (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., MCB supra; and Hong et al., PNAS supra) and/or SRC-1 (Spencer et al., Nature (1997) 389:194-198; Onate et al., .Science (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

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Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include TR-based disorders including cardiovascular disease, metabolic disorders. hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples, TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T₃.

Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

After the three dimensional structure of the cocrystal is determined, the structural information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

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5 solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in **Appendix 1**. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interative drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including members of the steroid/thyroid receptor superfamily, such as the receptors ER. AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

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that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR-α, human RAR-γ, human RXR-α, human PPAR-γ, human PPAR-β, human PPAR-γ, human PR, human PR, human PR, human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2. A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong et al. (PNAS <u>supra</u>; and MCB <u>supra</u>), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR-α or Glu 202 to Asp 461 of the human TR-β.

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

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To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

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components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the handing drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., <u>supra</u>. The structure is refined following standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

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EXAMPLES

Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators

A. Human TRβ LBD

Human TRB LBD (His6-E202-D461) was expressed and purified as described (Shiau et al., Gene (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28) in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for 24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl, 10% glycerol, 25mM ß-merceptoethanol and 0.1mM PMSF as described above. The lysate was cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an imidazole gradient (12 - 300 mM). TRB LBD containing fractions were loaded in 0.6M ammonium sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium sulfate gradient [0.6 - 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TRB LBD were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T₃ (Sigma). The hydrophobic interaction run was repeated with liganded receptor under the same conditions. Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed to 20mM Hepes pH7.0, 3mM DTT and 0.1 μ M T₃ using NAP columns (Pharmacia). For crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10 concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter bacterial culture.

B. Human TR mutants

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded oligonucleotides which encode the mutant sequence and which have ends allowing them to be ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PfiMI, BstXI, BseRI, BsmFI, PvuII, NspI, SmaI, PmII, BglII and BsmI restriction sites of the hTRβ1 cDNA sequence, or the 3' plasmid polylinker SalI, or BamHI restriction sites. The hTRβ1 sequences thus mutated were subcloned into the pCMX vector encoding the full-length 461 amino acid hTRβ1 sequence. Some of the mutations of the hTRβ1 in the CMX vector and all three mutations of the hERα in the pSG5-ER-HEGO vector (Tora et al., EMBO (1989) 8:1981) were created using Quick Change Site-

Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

C. Human ERa LBD

The human ERα-LBD 297-554 was overexpressed as described previously (Seielstad, et al., supra) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained the sequence Met-Asp-Pro fused to residues 297 to 554 of the hERα (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., Proc. Natl. Acad. Sci. USA (1980) 77:5115-5119; Landel, et al., Mol. Endocrinol. (1994) 8:1407-1419; Landel, et al., J. Steroid Biochem. Molec. Biol. (1997) 63:59-73).

To carboxymethylate the solvent-accessible cysteines, the bound hERα-LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., Steroids (1996) 61:367-373). Protein was eluted with 3 x 10-5 M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hERα-LBD was typically close to 100% (Seielstad, et al., Biochemistry (1995) 34:12605-12615). The affinity-purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hERα-LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass spectrometry.

D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ERα LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ³⁵S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

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³⁵S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hERα LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376; L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

E. Human ER LBD-GST Fusion Protein

A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hERα was constructed by subcloning the EcoRI fragment from pSG5 ERα-LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

F. Radiolabeled full-length receptors and coactivator proteins

Wild-type (WT) or mutant pCMV-hTRβ1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [35 S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTRβ1 (full-length, WT or mutants, WT provided by. C. Costa), and the GST-hRXRα (full-length

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provided by. C. Costa), fusion proteins were produced in E. coli strain HB101 as per the 5 manufacturer's protocol (Pharmacia Biotech).

G. Coactivator GRIP1 563-767 His6 GST fusion protein

GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX 10 GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freezethawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquts and stored at −70°C.

H. Coactivator GRIP1 563-767 His6

GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived fron pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

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5 pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

Example 2: Peptide synthesis

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Coactivator peptides were obtained using standard techniques. All peptides were HPLC purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ($A_{276} = 1450 \text{ M-1cm-1}$) or by amino acid analysis following standard techniques.

Example 3: Binding assays with nuclear receptors and coactivators

A. GST-GRIP Pull-down Assays and Peptide Competition Assays

Binding experiments were performed by mixing glutathione beads containing 10 μg of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2 μl of the [35S]-labeled wild-type or mutant hTRβ1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150 μl of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM MgCl₂, 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the presence or absence of 1 μM T₃. Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [³⁵S]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were performed in the presence and absence of 10µM dexamethasone or 1µM RU486 for GR and 10µM triiodothyronine for TR. Expression was quantified by phosphoimager analysis (BAS2000, Fuji). For all binding assays 50µl of a 20% bead suspension containing either 1.6 or 4.0 µM bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2µl or 1.4µl *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding buffer described above supplemented with 20 µg/ml BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200µl binding buffer + BSA at 4°C before elution of the bound proteins in 20µl SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was determined by phosphoimager analysis.

B. GST-hTRβ1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [³⁵S]-labeled full-length GRIP1, [³⁵S]-labeled full-length SRC-1a, and [³⁵S]-labeled full-length hRXRα, to GST-hTRβ1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and E457K all bound to hRXRα with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [³⁵S]-Met-labeled full-length hTRβ1 WT and mutants (data not shown).

20 C. <u>GST-hERα LBD Pull-down Assays</u>

The wild-type and mutant GST-hERα LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hERα (H222). Cleared extracts containing the GST- hERα LBDs were incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μM of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μl glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. ³⁵S-labeled GRIP1 was synthesized by *in vitro* transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hERα LBDs were incubated for 2.5 hours with 2.5 μl aliquots of crude translation reaction mixture diluted in 300 μl of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,

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5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound ³⁵S-GRIP1 was quantitated by fluorography following SDS-PAGE.

D. <u>Electrophoretic Mobility Shift Assays</u>

GRIP1, a mouse p160 coactivator, recognizes the ER α LBD in a ligand-dependent manner. The binding of agonists to the ER α LBD promotes recruitment of GRIP1, whereas binding of antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER α strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER α LBD in the presence of either DES or OHT. Eight microgram samples of purified hER α -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10 μ l of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

In the presence of the NR-box 2 peptide, the migration of the DES-hERα-LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hERα-LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

Example: 4 Transfection assays with TR and hERa

HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5 μg of the reporter p(DR-4)₂ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results (data not shown). Also, 2 μg of the hTRβ1 expression vector, pCMX-TR (WT or mutant), and 0.5 μg transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the β-galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

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5 or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., supra), and GC cells expressing TR (Norman et al., J. Biol. Chem. (1989) 264:12063-12073).

For hERa assays, 5 µg of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, et al., Mol Cell Biol. (1995) 15:1554), 0.5 µg expression vector encoding full-length hER α , pSG5-er HEGO (WT or mutants), and 2 μg of pj3lacz, were used. For the experiments of Figures 2 and 4, 0.5 µg of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1 μM T₃ or E₂, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the β -galactosidase activities were also assayed to correct for differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

Example 5: Hormone binding assays for wild-type and mutant TRs

The T₃ binding affinity constants (Kd) for in vitro -translated WT and mutant TRs were measured using $[^{125}I]$ 3,5,3' triiodo-L-thyronine ($[^{125}I]T_3$) in gel filtration binding assays as described (Apriletti et al., Protein Expr. Purif. (1995) 6:363). Both the Kd and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81 ± 12 pM. The relative affinity was determined by dividing the WT Kd by each mutant Kd. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3.5,3'-triiodo-L-thyronine (T₃) bind equally well to the coactivator. GRIP1. In all cases. GRIP1 binding was hormone-dependent

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5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (Figure 1). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (Figure 1). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators recognize the same TR surface residues.

Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T₃ increased reporter gene activity 5-fold in cells expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in Figure 1. By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T₃ which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of GRIP1 binding and activation (Figure 2). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

Example 8: Effect of TR mutations on other receptor functions

The effects of the mutations on other receptor functions also were examined. All of the mutants bound radiolabeled thyroid hormone (Kd values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T3—dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al.. *supra*), suggesting that the CBS residues do not participate in TR actions mediated through these proteins. These data

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indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

Example 9: Coactivator binding site in ER

Three separate mutations (K362A, V376R, and E542K) were created in human estrogen receptor-α (hERα) which align to three of the effective positions in hTRβ1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which responds to the ER amino-terminal activation function (Berry et al., EMBO J (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

Example 10: Coactivator NR-box binding affinity for TR

To study the interaction between nuclear receptors and GRIP1 in vitro, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTRB LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = $1.0~\mu$ M) over NR-box 3 (EC50 = $4.0~\mu$ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

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Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

Example 11: Coactivator NR-box binding affinity for GR

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (**Figure 8**). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

Example 12: Coactivator peptide binding affinity for TR

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTRß LBD were performed using coactivator peptides containing different NR- boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLLQDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBDß with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of GRIP1 with hTRß LBD only at very high concentrations (EC50 = 130 μ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTRß LBD for NR-box 2 (EC50 (NR-box 2) = 1.5 μ M, EC50 (NR-box 3) = 4 μ M). The apparent affinities (EC50) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the sequence and independent of the structural context of the NR-boxes.

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Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

Example 13: Binding affinity of TR for extended coactivator peptides

Sequence identity between all three central NR-boxes of the p160 coactivator family is limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (Figure 6). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTRB LBD were compared (Figure 10).

A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adiacent sequences.

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Example 14: Binding affinity of TR and GR for mutant coactivator

A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRLL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (Figure 11). Surprisingly, replacement of any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTRB LBD, it appears that their contribution to the affinity of NR-box 2 for hTRB LBD is cooperative rather than additive.

Similar results were obtained by competing the interaction of hTRB LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (Figure 11). Whereas the peptides containing the IL or LL replacement failed to interact with the hTRB LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (Figure 11). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTRß LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767) with hTRB LBD.

B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTRß LBD:NR-box 2 interaction surface, whereas the non conserved

isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTRB LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-KHKILHRLLQDSS-698 is highly complementary to the corresponding binding site in the hTRB LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., Nat Struct Biol. (1996) 3:87-94; Wagner et al., supra; Renaud et al., Nature (1995) 378:681-689; Bourguet et al., Nature (1995) 375:377-382; and Brzozowski et al., Nature (1997) 389:753-758).

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic alphahelices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL) differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a

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GRIP1 mutant lacking NR-box 3, binds GR in vivo (Ding et al., <u>supra</u>). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

C. TR affinity for residues adjacent to ILxxLL motif

Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (Figure 11). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

Example 15: Crystallization and Structure Determination of NR LBD Complexes

A. Crystallization of hTRB LBD with T₃ and GRIP1 NR-box 2 Peptide

Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the 30 hTRB LBD. The complex of the hTRB LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTRB LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding

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of prepared drops with microcrystals of the hTR\$ LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTR\$ LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTR\$ LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTR\$ LBD, residues K211-P254 and G261-D461 of monomer 2 of the hTR\$ LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-KILHRLLQDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLLQD-696 (Appendix 1).

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Briefly, the complex between the hTRß LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal) volumes of a solution of 9mg/ml hTRß LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTRß LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10-3 to 10-5 dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTRß LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

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Table 1

Data collection, phasing, and refinement statistics

			Dat	a collection	1	
Data set		lution A)	Reflect	ions	Coverage (%)	R _{sym}
Native	3	.6	measured 35565	unique 8490	96.3	0.007
			Rot	ation searc	h	
Search model		Euie	r angles (°)		Соттеватіс	on coefficient
		Θ,	Θ ₂	Θ,	Highest peak	Highest false pea
hTR β LBD	Mi	60.12	80.68	241.90	16.3	
<u> </u>	M2	9.93	87.70	180.6	15.9	14.2
			Tran	slation sear	-ch	
	ļ	F	ractional coor	dinates	Trans	slation function
		x	У	z	Highest peak (o)	Highest false peak (o
	Mi	0.522	0.428	0.250	19.52	10.02
	M2	0.200	0.932	0.119	26.11	5.77
			R	efinement		
	Res	solution (Å)	Refi	ection	R	R _{free}
F > 2(25 - 3.7	76	14	0.2990	0.3219
All data		25 - 3.7	7.	851	0.3010	0.317

 $R_{\text{sym}} = \sum_{h} \sum_{i} |I_{h,i} \hat{\mathbf{u}} (I_{h}(|/\Sigma I_{h} \text{ for the intensity } (I) \text{ of } i \text{ observations of reflection } h.$ Correlation coefficient = $\sum_{h} Eo^{2}Ec^{2} - Eo^{2}Ec^{2} / \left[\sum_{h} (Eo_{2} - Eo^{2})^{2} \sum_{h} (Ec^{2} - Ec^{2})^{2}\right]^{1/2}$

Translation function $(t_a, t_b, ...) = \Sigma_h (|Eo_{(h)}|^2 - \Sigma_h < |Eo_{(h)}|^2 >) (Ec_{(h,t_a,t_b,...)}|^2 - < |Ec_{(h)}|^2)$ where E_o represents the normalized observed structure factor amplitudes, and E_c represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation (t_a, t_b) of the NCS monomers, divided by the rms value of the translation function density.

R factor = $\Sigma | F_{\text{obs}} - F_{\text{calc}}| / \Sigma | F_{\text{obs}}|$.

R_{free} is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

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B. Crystallization of hERa LBD with DES and GRIP1 NR-box 2 Peptide

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Crystals of a DES-hERa LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hERa LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two µL samples of this solution were mixed with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μL of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2₁ with cell dimensions a=54.09, b=82.22, c=58.04 and β=111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200 μm x 40 μm x 40 μm crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μM peptide and frozen in an N₂ stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., Methods Enzymol. (1997) 276:307-326) using the default -3 σ cutoff.

C. Crystallization of hERa LBD with OHT

Crystals of the hER α LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μ L) of a solution containing 3.9 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6₅22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit consists of a single hER α LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μ m x 250 μ m x 40 μ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N₂ suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

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5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski. et al., <u>supra</u>) using the default -3σ cutoff.

Example 16: Structure determination and refinement of NR LBD complexes

A. Structure of hTRB LBD with T₃ and GRIP1 NR-box 2 Peptide

Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In Macromolecular Crystallography, Part A (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in AMORE from a model of hTRB LBD with the ligand, T3, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTRB LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTRB LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and conventional difference Fourier maps for the iodine atoms of the T3 ligand confirmed the correctness of the solution. The iodine atoms for both T3 ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTRß LBD. The electron density could be modeled as a short α -helix, and the observed side chain density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTRB LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTRB LBD:GRP1 site 2 peptide complex are attached as Appendix 1.

B. Structure of hERa LBD with DES and GRIP1 NR-box 2 Peptide

Initial efforts to determine the structure of the DES-hER\alpha LBD-NR box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4")

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5 suite: programs for protein crystallography", Acta Crystallogr. (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RAR? LBD (Renaud, et al., supra) as the search probe (R=58.2%, CC=35.6% after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 Å between this model and the final model based on $C\alpha$ positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., Bull. Soc. Chim. Belg. (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., Acta Crystallogr. (1997) D53:240-255) (using tight NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 Am. Cryst. Assoc. Mtg. Abstr. (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of weights.

However, although the DES-hER α LBD-NR complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hERα LBD-NR-box 2 peptide complex became available when the R_{free} of the OHT-hER α LBD model was ~31%. Both monomers in the asymmetric unit of the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER α LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximumlikelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 Å (with no σ cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER α

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5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% (R_{free}=25.0%) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The γ-carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 377, the γ-carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ERα LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of DES-LBD-peptide complex are attached as **Appendix 2**.

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5 Table 2 Summary of Crystallographic Statistics Ligand Data Collection DES **OHT** Space group $P2_1$ P6522 10 Resolution 2.03 1.90 Observations 104189 269253 Unique 30265 23064 Completeness (%) 98.4 99.1 $R_{\text{sym}}(\%)^{a}$ 7.8 7.0 15 Average I/σI 9.8 16.1 Refinement Number of non-hydrogen atoms 4180 2070 R_{cryst} (%)^b/ R_{free} (%) 19.9/25.0 23.0/26.1 20 Bond r.m.s. deviation (Å) 0.006 0.006 Angle r.m.s. deviation (°) 1.05 1.05 Average B factor (Å²) 34.0 40.4 $R_{\text{sym}} = \sum_{i} |I_{i} - \langle I_{i} \rangle| / \sum_{i} I_{i}$ where $\langle I_{i} \rangle$ is the average intensity over symmetry equivalents 25 $R_{\text{cryst}} = \sum |F_o - F_c| / \sum |F_o|$

C. Structure of hERa LBD-OHT complex

The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6₁22 and P6₅22. A translation search in P6₅22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR

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5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the R_{free} set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no σ cutoff) were included. The final model consisted of residues 306-551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hERα LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% (R_{free}=26.2%). Atomic coordinates of OHT-hERα LBD complex are attached as **Appendix 3**.

Example 17: Structural analysis of hTRB LBD:GRIP 1 NR-box 2 peptide complex

A. Structure of cocrystal complex (contents of asu)

The asymetric unit (asu) of the crystal contains two monomers of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (Figure 12). The structure of the hTR β LBD, which closely resembles that of the rTR α LBD (Wagner et al., *supra*), consists of twelve alpha-helices and two β -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR β LBD and the rTR α LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic α -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

The relation of the two monomers of the hTR\$ LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., <u>supra</u>; Brzozowski et al., <u>supra</u>). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the alpha-helix of the cocrystal peptide contacts monomer 1 of the hTR\$ LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

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B. Structure of the GRIP1 NR-box 2 peptide

The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLLQDSS-698). For the NR-box 2 peptide in monomer 1 15 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the 20 GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., Science (1996) 274:948-953), VP16:TAF31 (Uesugi et al., Science (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan 25 et al., Cell (1997) 91:741-752).

C. Structure of the hTRB LBD:GRIP1 NR-box 2 peptide interface

The hTRß LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

The GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

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defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTRB LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

Example 18: Overall Structure of the DES-hERα-LBD-NR-box 2 Peptide Complex

The asymmetric unit of the DES-hERa LBD-NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E2 and RAL (Brzozowski, et al., supra and Tanenbaum, et al., supra). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar structures (r.m.s.d. 0.47 Å based on Ca positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E₂ (Brzozowski, et al., supra); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix. Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

Example 19: Structure of the OHT-hERa LBD Complex

The binding of OHT induces a conformation of the hER α LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

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complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., supra).

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Example 20: Coactivator binding site structure and function

A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., Figures 5, 14, and 15). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453, L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

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mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ERα LBD buries 1000 Å² of predominantly hydrophobic surface area from both molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization of the binding site of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ERα LBD, which is the same NR-box 2 peptide utilized to crystallize the T₃-TR

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LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter. These residues are highly conserved among the nuclear receptor super family (Figure 19). Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of exploiting the slight differences among the coactivator binding sites of nuclear receptors in designing and identifying compounds that target specific nuclear receptors.

The ERα LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) α helix formed by the side chains of Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689 and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile 689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix project away from the ERα receptor and either interact predominantly with solvent or form symmetry contacts. None of the side chains of the polar and charged residues outside the helical region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is involved in hydrogen bonds or salt bridges with its associated ERα LBD monomer. The ε-amino group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-terminal three residues of peptide B are displaced from monomer B and interact extensively with a symmetry-related ERα LBD.

In addition to interacting with the hydrophobic face of the peptide helix, the ERα LBD stabilizes the main chain conformation of the NR box peptide by forming capping interactions with both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These interactions position the stabilizing charges of the γ-carboxylate of Glu 542 and ε-amino group of Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

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hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the ε-amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

Except for the orientation of helix 12, the structure of the peptide binding groove of the ER α LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) <u>LLEML</u> instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its ε -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu 380. The Glu 380 γ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER α LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

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OHT complex buries more solvent accessible surface area (\sim 1200 Å²) than the NR box peptide in the DES-ER α LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator proteins to nuclear receptors for all members of the nuclear receptor super family.

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All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

Appendix 1

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Atomic Coordinates for Human TR-B Complexed With T3, and a GRIP1 NR-box 2 Peptide

```
REMARK full length numbering
      REMARK all residue names correct
 10
      REMARK peptide sequence
      REMARK two molecules of TRB - CHAIN A and CHAIN B
      REMARK two molecules of T3 - CHAIN J and CHAIN K
      REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y
 15
      REMARK chain X lies between A and B
     REMARK chain Y interacts with B only
     REMARK residues differing between A and B include:
     REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains)
     REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains)
 20
     REMARK additionally Gly 261, Gly 262 are not visible in chain A
     REMARK residues differing between X and Y include:
     REMARK A 692 Arg
     REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698
     REMARK are not visible in chain Y
 25
     ATOM
               1
                  N
                       LYS A 211
                                      52.546 23.912
                                                      35.239
                                                               1.00 45.76
                                                                            7
     ATOM
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                                              24.345
                                                      36.586
                                                               1.00 43.42
                                                                            6
     MOTA
               3
                       LYS A 211
                  С
                                      52.035
                                              23.665
                                                      37.836
                                                               1.00 35.68
     MOTA
               4
                  0
                       LYS A 211
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                                              22.556
                                                      37.763
                                                               1.00 33.58
                                                                            8
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               5
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                                              25.825
                                                      36.779
                                                              1.00 46.72
                                                                            6
30
     MOTA
               6
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                       PRO A 212
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                                                               1.00 35.64
                                                                            7
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               7
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                                              25.474
                                                      39.842
                                                               1.00 38.60
                                                                            6
     MOTA
               8
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                      PRO A 212
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                                                      40.166
                                                              1.00 38.35
                                                                            6
     MOTA
               9
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                                                      41.440
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                                                      41.255
                                                              1.00 42.00
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                                                              1.00 45.16
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40
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                                                      37.601
                                                              1.00 47.60
                                                                            6
     ATOM
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                                                      36.353 1.00 50.68
                                                                            6
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                                                              1.00 45.96
                                                                           6
45
    ATOM
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                      GLU A 213
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                                                              1.00 46.44
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              24
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                                                      41.596
                                                              1.00 47.52
                                                                           6
    MOTA
              25
                  CB
                     PRO A 214
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                                                     40.816
                                             19.629
                                                              1.00 45.40
                                                                           6
50
    ATOM
              26 CG
                     PRO A 214
                                     43.588
                                             19.674
                                                      39.327
                                                              1.00 49.89
                                                                           6
    ATOM
              27 C
                      PRO A 214
                                     44.787
                                             19.082
                                                      42.625
                                                              1.00 45.70
                                                                           6
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                                     45.816
                                             18.466
                                                     42.535
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                                             18.876
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                                                             1.00 45.24
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                                                                           6
55
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             31
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                     THR A 215
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                                                     46.093
                                                             1.00 44.86
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    MOTA
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                 CG2 THR A 215
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                                             16.995
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                                                             1.00 52.51
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5	ATOM	35	0	THR A	215	41.816	17.501	44.691	1.00 53.48	8
-	MOTA	36	N	ASP A	216	43.118	15.683	44.607	1.00 58.81	7
	MOTA	37	CA	ASP A	216	41.973	14.740	44.615	1.00 61.51	6
	MOTA	38	CB	ASP A	216	42.386	13.451	45.343	1.00 70.57	6
	ATOM	39	CG	ASP A	216	42.399	12.283	44.475	1.00 78.07	6
10	ATOM	40	OD1	ASP A	216	41.532	12.161	43.586	1.00 82.31	8
	ATOM	41	OD2	ASP A	216	43.293	11.436	44.684	1.00 86.55	8
	MOTA	42	С	ASP A	216	40.640	15.311	45.268	1.00 58.42	6
	ATOM	43	0	ASP A	216	39.598	14.840	44.924	1.00 56.85	8
	ATOM	44	N	GLU A	217	40.673	16.270	46.217	1.00 54.92	7
15	MOTA	45	CA	GLU P	217	39.502	16.937	46.856	1.00 53.37	6
	MOTA	46	CB	GLU A		39.943	17.459	48.216	1.00 51.02	6
	MOTA	47	С	GLU A		39.113	18.144	45.956	1.00 53.55	6
	MOTA	48	0	GLU F		37.905	18.394	45.695	1.00 54.33	8
	MOTA	49	N	GLU A		40.162	18.895	45.511	1.00 49.20	7
20	ATOM	50	CA	GLU A		39.933	20.073	44.661	1.00 45.94	6
	ATOM	51	CB	GLU A		41.232	20.855	44.304	1.00 43.43	6
	MOTA	52	CG	GLU A		41.907	21.579	45.479	1.00 40.86	6
	MOTA	53	CD	GLU A		43.061	22.446	45.074	1.00 39.88	6 8
	ATOM	54	OE1			43.895	22.019	44.232	1.00 37.61	8
25	MOTA	55	OE2			43.183	23.583	45.599 43.390	1.00 34.01 1.00 44.71	6
	MOTA	56	С		A 218	39.249	19.647	43.390	1.00 44.71	8
	MOTA	57	0		A 218	38.302	20.291 18.553	42.797	1.00 44.02	7
	ATOM	58	N		A 219	39.720	18.061	41.574	1.00 44.02	6
	MOTA	59	CA		A 219	39.109 39. 7 99	16.793	41.074	1.00 48.42	6
30	ATOM	60	CB		A 219 A 219	40.879	17.029	40.141	1.00 54.61	6
	MOTA	61	CG	TRP		40.755	17.256	38.733	1.00 55.24	6
	ATOM	62 63	CE2		A 219	42.067	17.523	38.245	1.00 53.67	6
	ATOM ATOM	64	CE3		A 219	39.691	17.234	37.828	1.00 54.55	6
35	ATOM	65	CD1		A 219	42.159	17.159	40.447	1.00 55.75	6
33	MOTA	66	NE1		A 219	42.895	17.485	39.339	1.00 54.43	7
	MOTA	67		TRP		42.330	17.851	36.895	1.00 52.54	6
	ATOM	68		TRP		39.943	17.535	36.509	1.00 55.17	6
	ATOM	69	CH2		A 219	41.239	17.820	36.029	1.00 55.59	6
40	ATOM	70	C		A 219	37.646	17.743	41.812	1.00 47.32	6
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	ATOM	72	N	GLU	A 220	37.376	17.142	42.965	1.00 49.91	7
	ATOM	73		GLU	A 220	36.021	16.769	43.316	1.00 53.57	6
	MOTA	74	СВ	GLU	A 220	36.052	16.055	44.649	1.00 58.18	6
45	ATOM	75	CG	GLU	A 220	35.149	14.930	44.672	1.00 73.13	6
	ATOM	76	CD	GLU	A 220	35.735	13.935	45.442	1.00 80.06	6
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	MOTA	78	OE:	2 GLU	A 220	35.078	13.478	46.378	1.00 82.78	8
	ATOM	79	С	GLU	A 220	35.161	18.026	43.381	1.00 50.51	6
50	ATOM	80	0		A 220	33.991	18.010	42.995	1.00 49.94	8
	ATOM	81	N	LEU	A 221	35.761	19.120	43.865	1.00 43.71	7
	ATOM	82	CA		A 221	35.047	20.398	43.951	1.00 42.81	6
	ATOM	83	CB		A 221	35.935	21.510	44.510	1.00 39.21	6
	ATOM	84			A 221	35.375		44.353	1.00 36.34	6
55	MOTA	85			A 221	33.941		44.836	1.00 36.93	6
	ATOM	86			A 221	36.226		45.122	1.00 24.18 1.00 43.46	6 6
	ATOM	87			A 221	34.563		42.575	1.00 43.46	8
	MOTA	88	0	LEU	A 221	33.392	21.104	42.395	1.00 45.25	0

5 ATOM 89 N ILE A 222 35.498 2J.871 41.628 ATOM 90 CA ILE A 222 35.192 21.226 40.254 ATOM 91 CB ILE A 222 36.379 20.997 39.343 ATOM 92 CG2 ILE A 222 35.970 21.182 37.893 ATOM 93 CG1 ILE A 222 37.532 21.922 39.707 ATOM 94 CD1 ILE A 222 38.804 21.586 39.004 ATOM 95 C ILE A 222 38.804 21.586 39.004 ATOM 96 O ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750 ATOM 98 CA LYS A 223 33.316 18.100 39.376	1.00 35.47 1.00 33.74 1.00 28.86 1.00 33.33 1.00 34.85 1.00 34.26 1.00 31.90 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	
ATOM 90 CA ILE A 222 35.192 21.226 40.254 ATOM 91 CB ILE A 222 36.379 20.997 39.343 ATOM 92 CG2 ILE A 222 35.970 21.182 37.893 ATOM 93 CG1 ILE A 222 37.532 21.922 39.707 ATOM 94 CD1 ILE A 222 38.804 21.586 39.004 ATOM 95 C ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 35.47 1.00 33.74 1.00 28.86 1.00 33.33 1.00 34.85 1.00 34.26 1.00 31.90 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	
ATOM 91 CB ILE A 222 36.379 20.997 39.343 ATOM 92 CG2 ILE A 222 35.970 21.182 37.893 ATOM 93 CG1 ILE A 222 37.532 21.922 39.707 ATOM 94 CD1 ILE A 222 38.804 21.586 39.004 ATOM 95 C ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 33.74 1.00 28.86 1.00 33.33 1.00 34.85 1.00 34.26 1.00 31.90 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	
ATOM 92 CG2 ILE A 222 35.970 21.182 37.893 10 ATOM 94 CD1 ILE A 222 37.532 21.922 39.707 ATOM 95 C ILE A 222 38.804 21.586 39.004 ATOM 96 O ILE A 222 34.067 20.365 39.735 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 28.86 1.00 33.33 1.00 34.85 1.00 34.26 1.00 31.90 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	
ATOM 93 CG1 ILE A 222 37.532 21.922 39.707 ATOM 94 CD1 ILE A 222 38.804 21.586 39.004 ATOM 95 C ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 98 CA LYS A 223 34.301 19.058 39.750	1.00 33.33 1.00 34.85 1.00 34.26 1.00 31.90 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	5 5 5 5 5
10 ATOM 94 CD1 ILE A 222 38.804 21.586 39.004 ATOM 95 C ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 33.33 6 1.00 34.85 6 1.00 34.26 6 1.00 31.90 8 1.00 39.49 7 1.00 44.43 6 1.00 50.81 6 1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	5 5 5 5 5
ATOM 95 C ILE A 222 34.067 20.365 39.735 ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 34.85 1.00 34.26 1.00 31.90 8 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 1.00 74.55	5
ATOM 96 O ILE A 222 33.033 20.873 39.319 ATOM 97 N LYS A 223 34.301 19.058 39.750	1.00 34.26 1.00 31.90 8 1.00 39.49 1.00 44.43 1.00 50.81 1.00 62.51 1.00 72.22 6 1.00 74.55	5
ATOM 97 N LYS A 223 34.301 19.058 39.750 ATOM 98 CA LYS A 223 32.315	1.00 31.90 8 1.00 39.49 7 1.00 44.43 6 1.00 50.81 6 1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	3
ATOM 98 CA LYS A 223 34.301 19.058 39.750	1.00 39.49 7 1.00 44.43 6 1.00 50.81 6 1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	;
ALOM 98 CA TVC 7 222 22 24 2-	1.00 44.43 6 1.00 50.81 6 1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	;
15 33.316 18.100 39.276	1.00 50.81 6 1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	,
99 CB LYS A 223 33.603 16.713 39 852	1.00 62.51 6 1.00 72.22 6 1.00 74.55 6	
ATOM 100 CG LYS A 223 32.741 15 631 39 227	1.00 72.22 6 1.00 74.55 6	
ATOM 101 CD TVS 2022	1.00 74.55 6	
ATOM 102 CF TVC 7 222	_	
ATOM 103 NZ TVS 2000	1 00	
20 ATOM 104 C TVS 7 222	1.00, 75.78 7	
ATOM 105 0 175 7 222 31.913 18.565 39.681	1.00 42.81 6	
ATOM 106 N TUD 222 30.936 18.323 38.984	1.00 40.36 8	
ATOM 107 CD 224 31.849 19.236 40.833	1.00 39.89 7	
ATOM 108 CD 700 30.602 19.792 41.378	1.00 39.93 6	
25 ATOM 100 271 30.805 20.206 42.851	1.00 40.57 6	
25 Million 109 OGI THR A 224 31.330 19 113 43 616	1.00 39.27 8	
ATOM 110 CG2 THR A 224 29.500 20.684 43 461		
ATOM III C THR A 224 30.167 21.011 40.533	_	
ATOM 112 O THR Ä 224 29.313 20.899 39.655		
ATOM 113 N VAL A 225 30 777 22 160 40 222	1.00 36.67 8	
30 ATOM 114 CA VAL A 225 30 532 23 426 40 132	1.00 38.02 7	
ATOM 115 CB VAT A 225	1.00 38.12 6	
ATOM 116 CG1 VAT A 225 21 512	1.00 38.19 6	
ATOM 117 CG2 VAL A 225	1.00 36.77 6	
ATOM 118 C VAL 225 32.343 24.464 41.505	1.00 41.76 6	
35 ATOM 119 0 VAL 7 225	1.00 37.52 6	
ATOM 120 N mys 223 29.119 23.803 38.239	1.00 36.77 8	
ATOM 121 C7 MUD 200 30.783 22.316 38.018	1.00-34.02 7	
ATOM 132 CB THE A 226 30.489 21.971 36.636	1.00 34.67 6	
31.565 20.999 36.083	1.00 30.56 6	
40 32.805 21.696 35.889	1.00 32.20 8	
124 CG2 THR A 226 31.108 20.346 34 783	1.00 20.99 6	
ATOM 125 C THR A 226 29.100 21.361 36 510		
ATOM 126 0 THR A 226 28.255 21.877 35.785		
ATOM 127 N ALA A 227 28.880 20 260 37 222		
ATOM 128 CA ALA A 227 27.602 19.562 37.204	1.00 39.20 7	
45 ATOM 129 CB ALA A 227 27 506 13.302 37.204	1.00 36.93 6	
ATOM 130 C ALA 227 26 503	1.00 38.06 6	
ATOM 131 O ALA A 227	1.00 37.69 6	
ATOM 132 N ALA A 229 26 211	1.00 40.94 8	
ATOM 133 CA ALA 200 20.811 21.630 38.107 1	1.00 32.86 7	
50 ATOM 134 CB 313 220 25.903 22.734 38.356 1	1.00 32.48 6	
ATOM 135 26.448 23.587 39.486 1	.00 28.25 6	
ATOM 135 C ALA A 228 25.732 23.570 37.101 1	.00 36.12 6	
AIA A 228 24.673 23.560 36 473 1		
ATOM 13 / N HIS A 229 26.782 24.306 36.752 1		
ATOM 138 CA HIS A 229 26.762 25.158 35.585 1		
33 ATOM 139 CB HIS A 229 28.155 25.691 35.366 1	.00 32.97 6	
ATOM 140 CG HIS A 229 28 250 26 333 33.200 1	.00 33.69 6	
ATOM 141 CD2 HIS A 229 29 025 26 081 32 020	.00 28.39 6	
ATOM 142 ND1 HTS 7 220	.00 28.83 6	
27.386 27.368 33.542 1	.00 30.47 7	

_		-	1	TO 2	220	27.654	27.692	32.280	1.00 26.95	6
5	MOTA	143	CE1 H			28.635	26.934	31.840	1.00 31.27	7
	ATOM	144	NE2 H	IS A		26.225	24.541	34.312	1.00 38.40	6
	ATOM	145		IS A		25.591	25.227	33.528	1.00 41.49	8
	ATOM	146		AL A		26.519	23.256	34.113	1.00 38.55	7
	ATOM	147		'AL A		26.088	22.554	32.916	1.00 40.40	6
10	ATOM	148		AL A		26.890	21.256	32.701	1.00 44.68	6
	MOTA	149	CB V			26.557	20.656	31.345	1.00 39.39	6
	MOTA	150	CG1 V			28.381	21.509	32.817	1.00 42.18	6
	ATOM	151		AL A		24.603	22.239	32.900	1.00 44.28	6
	ATOM	152		/AL A		23.959	22.316	31.847	1.00 45.94	8
15	ATOM	153 154		ALA A		24.072	21.862	34.059	1.00 45.59	7
	ATOM	155		ALA A		22.669	21.500	34.175	1.00 47.84	6
	ATOM	156		ALA A		22.482	20.582	35.374	1.00 45.08	6
	ATOM	157		ALA A		21.792	22.734	34.314	1.00 48.04	6
20	ATOM ATOM	158		ALA A		20.565	22.647	34.324	1.00 49.95	8
20	MOTA	159		THR A		22.436	23.894	34.384	1.00 47.26	7
	ATOM	160		THR A		21.722	25.161	34.528	1.00 43.64	6
	MOTA	161		THR A		22.112	25.832	35.850	1.00 41.93	6
	ATOM	162		THR A		23.467	26.283	35.791	1.00 39.10	8
25	ATOM	163			232	21.990	24.846	37.008	1.00.29.80	6
	ATOM	164			A 232	22.055	26.114	33.387	1.00 43.97	6
	ATOM	165			A 232	21.679	27.279	33.436	1.00 40.55	8 7
	MOTA	166			A 233	22.783	25.625	32.381	1.00 48.62	6
	MOTA	167			A 233	23.134	26.468	31.231	1.00 58.62 1.00 62.44	6
30	MOTA	168	CB		A 233	24.626	26.283	30.880	1.00 62.44	6
	MOTA	169	CG		A 233	25.141	27.355	29.927 30.096	1.00 65.50	8
	MOTA	170			A 233	24.822	28.544 26.951	28.959	1.00 03.30	7
	MOTA	171		ASN A	A 233	25.951	26.931	30.073	1.00 65.06	6
	MOTA	172			A 233	22.241 22.312	24.900	29.604	1.00 69.47	8
35	MOTA	173			A 233	21.381	26.954	29.646	1.00 68.80	7
	ATOM	174			A 234 A 234	20.423	26.708	28.564	1.00 70.98	6
	MOTA	175			A 234 A 234	19.748	28.015	28.186	1.00 71.43	6
	MOTA	176			A 234	20.988	26.062	27.308	1.00 73.83	6
40	ATOM	177			A 234	22.041	26.419	26.822	1.00 74.33	8
40	ATOM	178 179			A 235	20.227		26.819	1.00 75.07	7
	ATOM				A 235	20.562				6
	ATOM ATOM	180 181			A 235	20.328				6
	ATOM	182			A 235	18.887		23.908	1.00 77.07	6
45		183			A 235	17.896		25.019		6
73	MOTA	184			A 235	17.668	24.448	25.768		8
	MOTA	185			A 235	17.313	26.596			7
	ATOM	186			A 235	21.960	23.840			6
	ATOM	18			A 235	22.386				8
50		188			A 236	22.676				7
50	ATOM	189			A 236	24.053				6
	ATOM	19			A 236	24.923				6
	ATOM	19			A 236	24.917				8
	ATOM	19			A 237	25.739				
55		19		SER	A 237	26.566		_		
	ATOM	19		SER	A 237	27.981				
	ATOM	19			A 237	28.82				
	ATOM	19		SER	A 237	25.938	3 22.127	7 22.542	2 1.00 75.35	ð

5										
5		19			A 237	26.60	5 21.41	8 21.79 ⁻	7 1.00 75.47	, ,
	ATOM	19			A 238	24.64				-
	ATOM	19		HIS	A 238	23.84				
	ATOM	20		HIS	A 238	22.99				_
	MOTA	20		HIS	A 238	22.40				_
10	ATOM	20:	2 CD		A 238	22.79		_		
	ATOM	20:			A 238	21.22				_
	ATOM	204			A 238	20.95		-		
	ATOM	205	5 NE	2 HIS	A 238	21.874				
	ATOM	206	5 C		A 238	22.97		_		
15	ATOM	207			A 238					
	ATOM	208			A 239	21.863				
	ATOM	209			A 239	23.487		•		
	ATOM	210			A 239	22.872				6
	ATOM	211				23.563			1.00 81.77	
20	ATOM	212			A 239	25.022			1.00 89.67	
	ATOM	213			A 239	25.532		21.240	1.00 93.19	
	ATOM	213			A 239	26.961			1.00 95.46	
	ATOM				A 239	24.936		20.969		6
	ATOM	215			A 239	26.102		21.781	1.00 94.16	6
25	ATOM	216			A 239	27.268	27.241	21.475	1.00 97.48	7
23		217		TRP	A 239	27.798	29.598	20.764	1.00 96.23	, 6
	ATOM	218	_	TRP	A 239	25.763	30.967	20.569	1.00 96.75	6
	ATOM	219			A 239	27.171			1.00 97.32	
	ATOM	220			A 239	22.799	26.407		1.00 37.32	6
30	ATOM	221	0		Ä 239	21.706	26.562	19.263	1.00 70.77	6 8
30	ATOM	222	N		A 240	23.946	26.701	19.157	1.00 67.10	
	ATOM	223	CA		A 240	23.978	27.180	17.783	1.00 65.63	7
	ATOM	224	СВ		Ä 240	25.314	26.780	17.153	1.00 66.65	6
	ATOM	225	CG		A 240	26.529	27.342	17.872	1.00 69.83	6
2.5	ATOM	226	CD		A 240	27.805	27.037	17.108	1.00 09.83	6
35	ATOM	227	CE		A 240	28.980	27.720	17.776	1.00 71.49	6
	ATOM	228	NZ	LYS A	A 240	30.238	27.438	17.034	1.00 71.31	6
	ATOM	229	С	LYS A	A 240	22.808	26.699	16.895	1.00 72.23	7
	ATOM	230	0	LYS A	A 240	22.550	27.298	15.851		6
40	ATOM	231	N	ASN A	241	22.113	25.640	17.325	1.00 65.20	8
40	ATOM	232	CA	ASN A	241	20.976	25.078	16.599	1.00 66.69	7
	ATOM	233	CB	ASN A		21.122	23.562	16.550	1.00 67.53	6
	ATOM	234	CG	ASN A		22.304	23.121		1.00 67.98	6
	ATOM	235		ASN A		22.404	23.506	15.693	1.00 70.19	6
	ATOM	236		ASN A		23.176	22.310	14.503	1.00 71.37	8
45	ATOM	237		ASN A		19.570		16.271	1.00 71.48	7
	ATOM	238		ASN A		18.581	25.421	17.152	1.00 66.62	6
	ATOM	239		LYS A		19.475	24.822	16.731	1.00 64.76	8
	ATOM	240		LYS A		18.191	26.380	18.069	1.00.66.86	7
	ATOM	241		LYS A			26.786	18.642	1.00 67.46	6
50	ATOM	242		LYS A		18.164	26.396	20.119	1.00 67.93	6
	ATOM	243		LYS A		18.250	24.896	20.337	1.00 71.52	6
	ATOM	244		LYS A		17.004	24.149	19.821	1.00 74.32	6
	ATOM	245		LYS A		15.755	24.491	20.643	1.00 74.41	6
	ATOM	246				15.927	24.161	22.109	1.00 74.44	7
55	ATOM	247		LYS A		18.143	28.291	18.483	1.00 66.28	6
_	ATOM	248	7	LYS A		17.102	28.923	18.592	1.00 67.61	8
	ATOM	249		ARG A		19.334	28.813	18.204	1.00 64.19	7
	ATOM	250		ARG A		19.617	30.219		1.00 62.43	6
		200	CB A	ARG A	243	21.070	30.274		1.00 60.12	6

						23 665	31.636	17.305	1.00 40.00	6
5	MOTA	251		RG A		21.665	31.599	17.267	1.00 40.00	6
	MOTA	252		RG A		23.213		15.996	1.00 40.00	7
	ATOM	253		RG A		23.826	31.217		1.00 40.00	6
	ATOM	254		RG A		25.113	31.439	15.714	1.00 40.00	7
	ATOM	255		RG A		25.905	32.041	16.616	1.00 40.00	, 7
10	ATOM	256	NH2 F	ARG A	243	25.592	31.097	14.520		6
••	ATOM	257	C F	ARG A	243	18.639	30.789	16.950	1.00 62.97	
	ATOM	258	0 7	ARG A	243	18.662	30.390	15.784	1.00 63.96	8
	ATOM	259	N 3	LYS A	244	17.771	31.692	17.393	1.00 62.41	7
	ATOM	260		LYS A		16.790	32.309	16.498	1.00 61.57	6
15	ATOM	261		LYS A		15.368	31.974	16.962	1.00 63.68	6
13	ATOM	262		LYS A		15.102	30.471	17.104	1.00 71.29	6
		263		LYS A		13.641	30.167	17.468	1.00 73.83	6
	MOTA	264		LYS A		13.182	30.908	18.737	1.00 74.71	6
	ATOM			LYS A		13.951	30.536	19.970	1.00 73.32	7
	MOTA	265		LYS A		17.009	33.806	16.501	1.00 59.30	6
20	MOTA	266		LYS A		16.562	34.514	17.399	1.00 56.34	8
	MOTA	267				17.705	34.264	15.468	1.00 57.06	7
	MOTA	268		PHE À		18.045	35.692	15.333	1.00 59.01	6
	MOTA	269		PHE A		18.825	35.947	14.049	1.00 59.62	6
	MOTA	270		PHE A		19.908	34.979	13.834	1.00 66.60	6
25	MOTA	271	CG	PHE A		19.618	33.714	13.399	1.00 67.17	6
	MOTA	272		PHE P			35.309	14.139	1.00 69.25	6
	MOTA	273		PHE F		21.198	32.794	13.255	1.00 69.92	6
	MOTA	274		PHE F		20.614	34.385	13.233	1.00 70.50	6
	ATOM	275		PHE A		22.189	33.126	13.552	1.00 70.89	6
30	MOTA	276	CZ	PHE A		21.897	36.620	15.340	1.00 60.68	6
	ATOM	277	С		A 245	16.856		14.528	1.00 62.37	8
	MOTA	278	0		A 245	15.946	36.516	16.272	1.00 60.10	7
	MOTA	279	N		A 246	16.919	37.558	16.437	1.00 59.44	6
	MOTA	280			A 246	15.884	38.554	17.585	1.00 57.43	6
35	MOTA	281			A 246	16.227		18.086	1.00.54.41	6
	ATOM	282	CG		A 246	15.100		18.640	1.00 52.43	6
	ATOM	283	CD1		A 246	14.010			1.00 52.45	6
	ATOM	284	CD2		A 246	15.575				6
	ATOM	285	C		A 246	15.717				8
40	MOTA	286	0		A 246	16.706				7
	MOTA	287	N	PRO	A 247	14.473				6
	ATOM	288	CD	PRO	A 247	13.263			_	6
	MOTA	289) CA		A 247	14.198				6
	ATOM	290			A 247	12.687				6
45		293	L CG	PRO	A 247	12.161				6
	ATOM	292		PRO	A 247	14.996				
	ATOM	293		PRO	A 247	15.159				8
	MOTA	29		GLU	A 248	15.506	42.006			
	ATOM	29			A 248	16.280	43.197			
50		29			A 248	16.483	43.273			
50	ATOM	29			A 248	17.012	2 44.67	9.966		
	ATOM	29			A 248	16.98		9 8.471		
		29			A 248	16.43		7.644		
	ATOM	30			A 248	17.50				
, ,	ATOM	30			A 248	15.62				
55		30			A 248	16.29				
	ATOM				A 249	14.30				
	MOTA	30			A 249	13.49				3 6
	MOTA	30	4 CA	MOP	A 277	13.13				

5	ATOM	305	CB	ASP	A	249	12.088	45.531	12.116	1.00	62.97	6
	ATOM	306	CG	ASP	Α	249	11.277	44.527	12.870	1.00	64.63	6
	ATOM	307	ODl	ASP	A	249	11.687	43.352	12.963	1.00	64.84	8
	MOTA	308	OD2	ASP	A	249	10.183	44.880	13.395		66.52	8
	MOTA	309	С	ASP	A	249	13.371	46.062	14.130		64.31	6
10	ATOM	310	0	ASP	Α	249	13.310	47.250	14.468		64.73	8
	ATOM	311	N	ILE			13.274	45.049	14.997		63.09	7
	ATOM	312	CA	ILE			13.133	45.318	16.418		64.39	6
	ATOM	313	СВ	ILE			13.035	44.034	17.214		65.79	6
	ATOM	314	CG2	ILE			12.001	44.104	18.336		64.78	
15	ATOM	315	CG1	ILE			12.611	42.860	16.341			6
	ATOM	316	CD1	ILE			11.753	41.852	17.088		65.28	6
	ATOM	317	C	ILE			14.404	46.104			65.08	6
	ATOM	318	0	ILE			15.155		17.276		65.21	6
	ATOM	319	N	GLY				45.506	18.047		64.05	8
20	ATOM	320	CA				14.670	47.529	17.299		65.48	7
20		321		GLY			15.871	48.326	18.042		67.32	6
	ATOM		С	GLY			16.595	49.110	16.895		68.52	6
	MOTA	322	0	GLY			17.528	48.616	16.266		65.49	8
	ATOM	323	N	GLN			16.162	50.356	16.557		72.26	7
25	MOTA	324	CA	GLN			16.541	50.930	15.207		74.10	6
23	ATOM	325	СВ	GLN	•	•	15.316	50.844	14.295		75.82	6
	ATOM	326	С	GLN	•		16.995	52.403	15.084		77.17	6
	MOTA	327	0	GLN			17.572	52.955	15.986		76.50	8
	ATOM	328	N	ALA			16.374	53.372	13.908		80.78	7
30	MOTA	329	CA	ALA			16.687	54.725	13.567		83.70	6
30	ATOM	330	CE	ALA			16.381	54.956	12.093		83.23	6
	ATOM	331	С	ALA			16.159	55.960	14.345		85.59	6
	ATOM	332	0	ALA			15.317	56.721	13.798		85.69	8
	ATOM	333	N	PRO			16.384	56.155	16.264		35.05	7
35	ATOM	334	CD	PRO		-	17.102	55.053	16.908		33.97	6
33	ATOM	335	CA	PRO			16.002	57.231	17.219		35.89	6
	ATOM	336	CB	PRO			16.534	56.756	18.563		33.94	6
	ATOM	337	CG	PRO			17.146	55.441	18.349		33.31	6
	MOTA	338	С	PRO			16.717	58.498	16.731		37.75	6
40	ATOM	339	0	PRO	A	254	17.838	58.804	17.100	1.00	38.78	8
40	TER	•			_	0.60						
	ATOM	1	N	LYS			18.045	57.462	23.875		61.71	7
	ATOM	2	CA	LYS			16.824	56.712	24.215		64.36	6
	ATOM	3	CB	LYS			15.758	57.004	23.141		63.50	6
45	ATOM	4	С	LYS			16.841	55.180	24.429		63.41	6
45	ATOM	5	0	LYS			17.877	54.542	24.409		61.93	8
	ATOM	6	N	VAL		•	15.615	54.664	24.654		61.15	7
	ATOM	7	CA	VAL			15.292	53.229	24.856		59.46	6
	ATOM	8	CB	VAL			14.251	52.974	25.978		59.03	6
50	ATOM	9		VAL			14.229	51.494	26.368		53.79	6
50	ATOM	10		VAL			14.449	53.818	27.142	1.00	55.32	6
	ATOM	11	С	VAL			14.590	52.820	23.554	1.00	60.96	6
	ATOM	12	0	VAL			14.734	53.468	22.508	1.00	62.13	8
	MOTA	13	N	ASP			13.802	51.755	23.634	1.00	62.59	7
	MOTA	14	CA	ASP			12.995	51.263	22.526	1.00	64.95	6
55	ATOM	15	CB	ASP			13.825	51.077	21.271	1.00	64.32	6
	MOTA	16	CG	ASP			13.282	50.048	20.485	1.00	67.70	6
	MOTA	17		ASP			12.795	50.011	19.446	1.00	72.59	8
	ATOM	18	OD2	ASP	Α	265	13.354	48.867	20.294	1.00	68.84	8

5	ATOM	19	С	ASP	Α	265	1	12.326	49.9	43	22.952	1.00	65.64	6
	ATOM	20	0	ASP	Α	265	1	12.771	48.8	50	22.655	1.00	68.81	8
	ATOM	21	N	LEU	Α	266	3	11.256	50.19	52	23.702		65.12	7
	MOTA	22	CA	LEU	A	266	1	10.368	49.1	69	24.288	1.00	63.40	6
	ATOM	23	СВ	LEU	Α	266		9.115	49.9	38	24.708		67.34	6
10	ATOM	24	CG	LEU	Α	266		9.399	51.12		25.618		69.35	6
	ATOM	25	CD1	LEU				8.304	52.1		25.533		68.24	6
	ATOM	26		LEU				9.581	50.6		27.021		70.47	6
	ATOM	27	С			266		9.940	47.8		23.559	1.00		6
	MOTA	28	0			266		9.694	46.8		24.220		53.35	-8
15	MOTA	29	N			267		9.815	47.9		22.235	1.00		7
	ATOM	30	CA			267		9.417	46.6		21.572	1.00		6
	ATOM	31	CB			267		9.311	46.89		20.048	1.00		6
	ATOM	32	CG			267		9.129	45.49		19.322		62.89	6
	ATOM	33	CD	GLU				8.736	45.5		17.883		67.66	6
20	ATOM	34	OE1	GLU				9.433	46.2		17.080	1.00		8
	ATOM	35	OE2	GLU				7.710	44.9		17.503		69.40	8
	ATOM	36	С			267	7	10.504	45.68		21.895	1.00		6
	ATOM	37	0			267		10.255	44.48		21.988		58.34	8
	ATOM	38	N	ALA	-	-		1.712	46.2		22.054		53.43	7
25	ATOM	39	CA	ALA				12.903	45.4		22.374		49.00	6
	ATOM	40	СВ	ALA				14.137	46.2		21.983		45.72	6
	ATOM	41	С	ALA				12.908	45.19		23.873		45.76	6
	ATOM	42	0	ALA		•		12.887	44.0		24.307		41.50	8
	ATOM	43	N			269		2.918	46.2		24.663		41.43	7
30	ATOM	44	CA			269		12.920	46.19		26.118		43.96	6
	ATOM	45	СВ			269		12.395	47.42		26.777		40.10	6
	ATOM	46	CG			269		2.332	47.3		28.271		40.44	6
	ATOM	47	CD1	PHE				3.457	47.59		29.034		38.98	6
	ATOM	48	CD2	PHE				1.165	46.9		28.903		37.15	6
35	ATOM	49	CE1	PHE		-		3.409	47.40		30.436		32.12	6
	ATOM	50	CE2	PHE				1.105	46.8		30.303		38.41	6
	MOTA	51	CZ			269		2.228	47.0		31.071		40.55	6
	ATOM	52	С			269		2.017	45.0		26.520		49.76	6
	ATOM	53	0	PHE				2.277	44.32		27.484		52.15	8
40	ATOM	54	N			270		0.934	44.83		25.768		53.15	7
	ATOM	55	CA	SER				9.988	43.76		26.043		52.29	6
	ATOM	56	CB	SER	,			8.727	43.94		25.215		51.85	6
	ATOM	57	OG	SER				7.785	42.93		25.497		53.42	8
	ATOM	58	С	SER			1	0.637	42.46		25.685		49.38	6
45	ATOM	59	0	SER				1.068	41.74		26.562		48.74	8
	ATOM	60	N	HIS				0.683	42.17		24.383		50.15	7
	ATOM	61	CA	HIS				1.276	40.93		23.877		51.67	6
	ATOM	62	СВ	HIS				1.797	41.11		22.455		58.52	6
	ATOM	63	CG	HIS				0.775	40.88		21.399		68.97	6
50	ATOM	64		HIS				0.633	39.89		20.485		70.88	6
	ATOM	65		HIS			-	9.673	41.73		21.199		71.98	7
	ATOM	66		HIS				8.936	41.24		20.209		73.91	6
	ATOM	67		HIS				9.495	40.13		19.764		73.59	7
	ATOM	68	С	HIS			1	2.402	40.41		24.745		48.33	6
55	ATOM	69	0	HIS				2.707	39.22		24.743		48.39	8
	ATOM	70	N	PHE				3.029	41.33		25.487		41.34	7
	ATOM	71	CA	PHE				4.130	41.00		26.384		39.44	6
	ATOM	72	СВ	PHE				5.077	42.19		26.512		36.67	6
		. —					_	3.077	36.12	7 3	20.512	1.00	30.07	О

5	ATOM	73	3 CG	PHE A	A 272	15.953	3 42.413	3 35 300		
	ATOM	74		PHE A		16.619				-
	ATOM	75		PHE P		16.138				_
	ATOM	76		PHE P		17.454				_
	ATOM	77		PHE A		16.973				
10	ATOM	78		PHE A						
	ATOM	79		PHE A		17.634				
	ATOM	80		PHE A		13.650				
	ATOM	81		THR A		14.081				
	ATOM	82		THR A		12.756				7
15	ATOM	83		THR A		12.290				
	ATOM	84		THR A		11.651				6
	ATOM	85				10.442				8
	ATOM	86		THR A		12.601			1.00 49.73	
	ATOM	87		THR A		11.267			1.00 46.23	6
20	ATOM	88	-	THR A		10.854				8
2.0	ATOM			LYS A		10.849		28.440	1.00 46.21	7
		89		LYS A		9.871			1.00 54.53	6
	ATOM	90		YS A		9.414			1.00 54.36	6
	ATOM	91		YS A		10.498	37.015	28.515	1.00 56.88	6
25	ATOM	92		YS Ă		9.789		28.759	1.00 57.98	8
23	ATOM	93		LE A		11.836		28.491	1.00 56.48	7
	ATOM	94		LE A		12.609	35.746	28.767	1.00 52.64	6
	ATOM	95		LE A		13.444	35.346	27.543	1.00 49.15	6
	ATOM	96	CG2 I			12.568	34.829	26.429	1.00 47.42	6
20	ATOM	97	CG1 I			14.238	36.532	27.026	1.00 45.31	6
30	ATOM	98	CD1 I			15.001	36.242	25.771	1.00 37.22	6
	ATOM	99		LE A		13.541	35.870	29.982	1.00 51.78	6
	ATOM	100		LE À		14.014	34.873	30.503	1.00 49.80	8
	ATOM	101		LE A		13.790	37.107	30.415	1.00 51.76	7
25	ATOM	102		LE A		14.681	37.389	31.537	1.00 52.58	6
35	ATOM	103		LE A		14.691	38.877	31.844	1.00 55.04	6
	ATOM	104	CG2 I			13.311	39.340	32.261	1.00 53.28	6
	ATOM	105		LE À		15.675	39.206	32.976	1.00 57.31	6
	ATOM	106	CD1 I	LE A	276	17.096	38.942	32.655	1.00 60.32	
40	ATOM	107	C I	LE A	276	14.323	36.644	32.828	1.00 50.32	6
40	ATOM	108	O I	LE A	276	15.177	36.458	33.691	1.00 55.55	6
٠	ATOM	109	N T	HR A	277	13.072	36.209	32.963	1.00 47.33	8
	ATOM	110	CA TI	HR A	277	12.631	35.523	34.158	1.00 47.33	7
	ATOM	111	CB TH	HR A	277	11.098	35.456	34.217	1.00 42.39	6
	ATOM	112	OG1 TH	IR A	277	10.545	36.777	34.102		6
45	ATOM	113		IR A		10.657	34.838	35.539	1.00 46.38	8
	ATOM	114		IR A		13.211	34.118	34.304	1.00 37.17	6
	ATOM	115		IR À		13.796	33.796		1.00 39.84	6
	ATOM	116		OA.		13.055	33.790	35.365	1.00 40.55	8
	ATOM	117		OA:		12.370	33.534	33.288	1.00 38.20	7
50	ATOM	118		O A		13.595	31.894	32.023	1.00 36.34	6
	ATOM	119		OA		13.153		33.363	1.00 36.63	6
	ATOM	120		OA			31.244	32.064	1.00 32.95	6
	ATOM	121		OA		12.573	32.291	31.239	1.00 35.75	6
	ATOM	122		O A 2		15.101	31.932	33.476	1.00 38.60	6
55	ATOM	123		AA2		15.746	30.981	33.898	1.00 37.67	8
	ATOM	124		A A 2		15.656	33.051	33.035	1.00 37.05	7
	ATOM	125		A A 2		17.087	33.277	33.041	1.00 33.18	6
	ATOM	126		AA2 AA2		17.376	34.599	32.348	1.00 30.56	6
		•	~ AL	n # 2	. 13	17.624	33.312	34.452	1.00 33.47	6

							00 555	24 760	1.00 33.74	8
5	ATOM	127		LA A		18.523		34.789		7
	ATOM	128		LE A		17.060		35.260	1.00 29.96	6
	ATOM	129	CA I	LE A	280	17.459		36.646	1.00 25.94	
	MOTA	130	CB I	LE A	280	16.686	35.484	37.315	1.00 26.95	6
	ATOM	131	CG2 I	LE A	280	17.109	35.632	38.733	1.00 15.40	6
10	MOTA	132	CG1 I	LE A	280	16.931	36.808	36.595	1.00 26.73	6
	ATOM	133		LE A		16.292	38.002	37.272	1.00 34.31	6
	ATOM	134		LE A		17.263	33.066	37.412	1.00 31.39	6
	MOTA	135		LE A		18.116	32.679	38.207	1.00 35.69	8
	ATOM	136		CHR A		16.145	32.386	37.165	1.00 30.90	7
1.5		137		THR A		15.854	31.118	37.851	1.00 33.49	6
15	ATOM	138		THR A		14.598	30.413	37.277	1.00 37.18	6
	ATOM			THR A		14.795	30.099	35.898	1.00 46.48	8
	ATOM	139		THR A		13.352	31.281	37.444	1.00 32.85	6
	ATOM	140		THR A		17.045	30.176	37.713	1.00 29.94	6
	MOTA	141				17.478	29.546	38.684	1.00 25.55	8
20	MOTA	142		THR A		17.561	30.076	36.489	1.00 32.70	7
	MOTA	143		ARG A		18.692	29.198	36.218	1.00 34.27	6
	ATOM	144		ARG A		19.136	29.374	34.780	1.00 33.78	6
	MOTA	145		ARG A		19.130	28.086	34.013	1.00 45.15	6
	MOTA	146		ARG A		18.179	27.921	32.977	1.00 58.24	6
25	MOTA	147		ARG A		18.041	29.077	32.117	1.00 68.41	7
	MOTA	148			282	19.018	29.529	31.352	1.00 72.31	6
	ATOM	149			282		28.886	31.327	1.00 77.89	7
	ATOM	150			A 282	20.190	30.593	30.595	1.00 69.25	7
	MOTA	151			A 282	18.802	29.582	37.170	1.00 34.81	6
30	MOTA	152	С		A 282	19.823	28.735	37.855	1.00 36.03	8
	MOTA	153	0		A 282	20.380	30.882	37.190	1.00 31.71	7
	ATOM	154	N		A 283	20.135	31.434	38.057	1.00 30.16	6
	MOTA	155	CA		A 283	21.171	32.965	37.981	1.00 29.00	6
	MOTA	156	СВ		A 283	21.198	33.533	38.952	1.00 28.64	6
35	MOTA	157			A 283	22.208	33.415	36.578	1.00 28.28	6
	MOTA	158			A 283	21.525	30.992	39.498	1.00 32.50	6
	MOTA	159	С		A 283	20.942	30.717	40.229	1.00 33.48	8
	MOTA	160	0		A 283	21.879	30.717	39.892	1.00 30.96	7
	MOTA	161	N		A 284	19.671	30.527	41.239	1.00 29.14	6
40	MOTA	162	CA		A 284	19.289	30.865	41.548	1.00 31.27	6
	MOTA	163	CB		A 284	17.822		42.945	1.00 24.21	6
	ATOM	164		VAL	A 284	17.472		41.360	1.00 30.51	6
	MOTA	165			A 284	17.555		41.353		6
	MOTA	166			A 284	19.529				
45	ATOM	167	0		A 284	20.073		42.345		
	ATOM	168	N		A 285	19.121		40.327		
	ATOM	169	CA		A 285	19.277		40.306		
	ATOM	170	CB		A 285	18.586		39.072		
	ATOM	171	CG	ASP	A 285	17.083		39.149		
50	ATOM	172	OD1	ASP	A 285	16.484		40.110		
	ATOM	173	OD2	ASP	A 285	16.431		38.231		
	ATOM	174	С	ASP	A 285	20.751				
	ATOM	175		ASP	A 285	21.106				
	ATOM	176			A 286	21.604				
55		177			A 286	23.029				
55	ATOM	178			A 286	23.754	28.009			
	ATOM	179			A 286	25.252	28.027	38.987		
	ATOM	180			A 286	25.963		38.974	1.00 36.75	6
	711011	200				•				

5	ATOM	18	1 CD2	PHE	A 28	36	25.93	1 29.21	0 20 20	_	
	ATOM	18		PHE			27.33				
	ATOM	18			A 28						
	ATOM	18	_		A 28		27.30				
	ATOM	18			A 28		28.00				4 6
10		18					23.63			3 1.00 36.83	3 6
	ATOM	18			A 28		24.31				
					A 28		23.39	3 28.228	3 41.752	2 1.00 37.33	
	ATOM	188			A 28		23.91	7 28.448			
	ATOM	189			A 28		23.523				_
	ATOM	190		ALA	A 28	7	23.34				
15		19:		ALA	A 28	7	23.994			=	
	ATOM	192	2 N		A 28		22.114				
	ATOM	193	3 CA		A 28		21.429				
	ATOM	194	СВ		A 28						
	ATOM	195			A 28		19.994				
20	ATOM	196		LYS			19.025		•	1.00 51.43	6
	ATOM	197					17.628			1.00 60.23	
	ATOM	198		LYS			17.135	_	43.485		
	ATOM			LYS			17.196		42.268		
		199		LYS			22.120	24.632			
25	ATOM	200		LYS			21.967			1.00 45.66	
25	ATOM	201		LYS .			22.865		–	1.00 41.70	
	MOTA	202		LYS .	A 289	9	23.571				
	ATOM	203	CB	LYS .	A 289	9	23.655			1.00 40.67	6
	ATOM	204	CG	LYS 2			22.271		41.877	1.00 42.25	6
	MOTA	205	CD	LYS A			22.331		41.247	1.00 39.53	6
30	ATOM	206	CE	LYS				21.606	40.012	1.00 43.19	6
	ATOM	207		LYS A			20.941	21.362	39.447	1.00 45.74	6
	ATOM	208		LYS A			20.273	20.165	40.006	1.00 52.49	7
	ATOM	209		LYS A			24.948	23.185	44.003	1.00 41.50	6
	ATOM	210					25.642	22.184	44.080	1.00 39.77	8
35	ATOM	211		LEU A			25.312	24.370	44.490	1.00 40.68	7
	ATOM			LEU A			26.594	24.583	45.149	1.00 39.33	6
		212		LEU A			27.153	25.972	44.829	1.00 36.14	6
	ATOM	213		LEU A			27.358	26.290	43.365	1.00 34.81	6
	ATOM	214		LEU A			27.945	27.675	43.208	1.00 29.07	
40	ATOM	215	CD2	LEU A	290		28.267	25.242	42.757	1.00 23.07	6
40	ATOM	216	C :	LEU A	290		26.434	24.405	46.652		6
	ATOM	217		LEU A			25.803	25.235		1.00 40.08	6
	ATOM	218		PRO A			27.028	23.233	47.333	1.00 42.00	8
	ATOM	219	CD 1	PRO A	291		27.851		47.210	1.00 40.27	7
	ATOM	220		PRO A				22.330	46.519	1.00 39.65	6
45	ATOM	221		PRO A			26.905	23.096	48.659	1.00 38.28	6
	ATOM	222		PRO A			27.755	21.860	48.911	1.00 35.88	6
	ATOM	223					28.202	21.355	47.585	1.00 34.19	6
	ATOM	224		PRO A			27.327	24.298	49.522	1.00 40.05	6
	ATOM			PRO A			26.571	24.739	50.391	1.00 41.33	8
50		225		IET A			28.522	24.843	49.299	1.00 40.59	7
30	ATOM	226		IET A			29.021	25.957	50.097	1.00 42.86	
	ATOM	227	CB M	MET A	292		30.313	26.475	49.477		6
	ATOM	228		ET A			31.269	25.378		1.00 43.28	6
	ATOM	229		ET A			32.895		49.050	1.00 50.35	6
	ATOM	230		ET A				26.096	48.757	1.00 51.17	16
55	ATOM	231		ET A			33.812	24.647	48.074	1.00 54.63	6
	ATOM	232		ET A			27.984	27.066	50.149	1.00 41.05	6
	ATOM	233					27.986	27.886	51.057	1.00 39.66	8
	ATOM	234		HE A			27.080	27.078	49.172	1.00 39.30	7
		~ J 4	CA P	HE A	∠93		26.030	28.091	49.114	1.00 40.92	6
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						25.398	28.107	47.715	1.00 40.98	6
5	MOTA	235		HE A		24.348	29.168	47.524	1.00 42.78	6
	MOTA	236		HE A		24.546	30.493	47.747	1.00 44.40	6
	MOTA	237		PHE A			28.833	47.116	1.00 43.66	6
	MOTA	238		PHE A		23.071 23.701	31.478	47.564	1.00 39.83	6
	MOTA	239		PHE A			29.819	46.930	1.00 46.21	6
10	MOTA	240		PHE A		22.112	31.146	47.155	1.00 45.18	6
	MOTA	241		PHE A		22.430	27.772	50.164	1.00 45.54	6
	MOTA	242		PHE A		24.979	28.576	51.034	1.00 42.01	8
	ATOM	243		PHE A		24.686		50.062	1.00 47.05	7
	MOTA	244		CYS A		24.426	26.572	50.962	1.00 50.15	<i>.</i> 6
15	MOTA	245		CYS A		23.386	26.125	50.524	1.00 35.13	6
	MOTA	246		CYS A		22.944	24.733	48.829	1.00 43.50	16
	MOTA	247		CYS A		22.303	24.663	52.423	1.00 51.38	6
	ATOM	248		CYS A		23.825	26.125	53.322	1.00 53.83	8
	MOTA	249		CYS A		23.008	25.954	52.645	1.00 33.03	7
20	MOTA	250		GLU A		25.119	26.327		1.00 49.72	6
	MOTA	251		GLU A		25.666	26.384	53.996	1.00 57.40	6
	MOTA	252		GLU A		27.103	25.830	54.015	1.00 57.40	6
	MOTA	253		GLU A		27.182	24.309	54.061	1.00 69.63	6
	ATOM	254	CD	GLU A		26.660	23.747	55.342	1.00 78.43	8
25	ATOM	255		GLU F		27.291	23.946	56.412	1.00 82.82	8
	MOTA	256	OE2	GLU A		25.590	23.086	55.335 54.488	1.00 83.50	6
	MOTA	257	С	GLU A		25.653	27.831	55.426	1.00 48.54	8
	MOTA	258	0	GLU A		26.365	28.184	53.846	1.00 43.79	7
	MOTA	259	N	LEU A		24.804	28.631	54.159	1.00 45.42	6
30	MOTA	260	CA	LEU A		24.670	30.034	52.923	1.00 41.04	6
	MOTA	261	CB		A 296	25.062	30.864	52.315	1.00 42.74	6
	ATOM	262	CG		A 296	26.438	30.658	50.861	1.00 40.99	6
	ATOM	263		LEU Z		26.447	31.030 31.454	53.086	1.00 39.44	6
	ATOM	264		LEU		27.437	30.366	54.548	1.00 45.56	
35	MOTA	265	С		A 296	23.239	29.660	54.148	1.00 43.07	
	MOTA	266	0		A 296	22.301 23.050	31.405	55.365	1.00 46.99	
	MOTA	267	N		A 297	24.121	32.241	55.930	1.00 47.12	
	MOTA	268	CD		A 297	21.700	31.811	55.787	1.00 49.61	
	MOTA	269	CA		A 297	21.700		56.738	1.00 49.91	
40	MOTA	270			A 297	23.401	33.155	56.872	1.00 51.28	
•	MOTA	271	CG		A 297	20.864		54.558	1.00 49.59	
	ATOM	272			A 297	21.402		53.556		
	MOTA	273			A 297	19.545				
4.5	ATOM	274			A 298	18.618				
45	ATOM	275			A 298	17.201				
	MOTA	276			A 298	16.040				
	MOTA	277			A 298 A 298	18.583			and the second s	
	ATOM	278			A 298	18.039				
	ATOM	279				19.144				
50		280			A 299	19.179				
	MOTA	281			A 299	19.265				
	ATOM	282			A 299					
	ATOM	283			A 299	17.931				
	MOTA	284			A 299	17.613			_	
55		285			A 299	16.512				
	MOTA	286			A 299	18.436				
	ATOM	287			A 299	20.359				
	ATOM	288	3 0	GLU	A 299	20.269	5 37.441	. 52.573	, 1.00 4410	_

5	N TOM	20/								
-	ATOM ATOM	289	_		A 300	21.46	7 35.76	5 53.29	4 1.00 45.13	7 -
		290	_		A 300	22.66	1 36.04			
	ATOM	291			A 300	23.91	9 35.51			
	ATOM	292	_		A 300	24.22	3 36.23			_
10	ATOM	293			A 300	24.15				
10		294			A 300	24.57				
	ATOM	295			A 300	22.51				
	ATOM	296			A 300	22.77				
	ATOM	297			A 301	22.09				
1.5	ATOM	298			A 301	21.89				
15		299		GLN	A 301	20.99				
	MOTA	300		GLN	A 301	21.64				_
	ATOM	301		GLN	A 301	20.690				
	ATOM	302	OE1	GLN	A 301	19.658				
•	ATOM	303	NE2	GLN	A 301	21.027		-		
20	ATOM	304	С		A 301	21.242				7
	ATOM	305	0		A 301	21.482				6
	ATOM	306	N		A 302	20.413		_		8
	ATOM	307	CA		A 302	19.726				7
	ATOM	308	CB		A 302	18.502				6
25	ATOM	309	CG2		Ä 302	17.818				6
	ATOM	310	CG1	ILE	A 302	17.516		-	1.00 31.98	6
	ATOM	311	CD1		A 302	17.003			1.00 40.77	6
	ATOM	312	С		A 302	20.698			1.00 45.43	6
	ATOM	313	0		A 302				1.00 38.58	6
30	ATOM	314	N		A 303	20.960		-	1.00 40.81	8
	ATOM	315			A 303	21.228	37.972		1.00 37.50	7
	ATOM	316	СВ		A 303	22.179		- · -	1.00 39.33	6
	ATOM	317			A 303	23.023		50.109	1.00 39.06	6
	ATOM	318		TLE 2	A 303	23.946	40.522	49.861	1.00 36.19	6
35	ATOM	319			A 303	22.141	39.653	51.313	1.00 40.15	6
	ATOM	320			A 303	22.916	39.806	52.589	1.00 36.93	6
	ATOM	321			A 303	23.093	38.705	47.722	1.00 36.49	6
	ATOM	322			A 304	23.354	39.509	46.835	1.00 36.58	8
	ATOM	323			304	23.580	37.477	47.762	1.00 32.91	7
40	ATOM	324			A 304	24.465	36.964	46.734	1.00 27.55	6
	ATOM	325			304	24.935	35.554	47.123	1.00 22.35	6
	ATOM	326	CD1	LEU A	304	26.150	35.480	48.029	1.00 26.88	6
	ATOM	327	CD2	LEU A	304	26.267	36.731	48.876	1.00 24.82	6
	ATOM	328				26.084	34.226	48.861	1.00 23.69	6
45	ATOM	329		LEU A		23.764	36.968	45.389	1.00 28.05	6
	ATOM	330		LEU A		24.212	37.623	44.443	1.00 24.68	8
	ATOM	331		LEU A		22.657	36.236	45.318	1.00 26.34	7
	ATOM	332		EU A		21.892	36.147	44.089	1.00 30.91	6
	ATOM	333		EU A		20.565	35.434	44.359	1.00 32.50	6
50	ATOM			EU A		20.637	33.950	44.635	1.00 33.36	6
20	ATOM	334	CD1 L	EU A	305	19.247	33.370	44.779	1.00.33.87	6
		335	CD2 L			21.340	33.280	43.466	1.00 31.72	
	ATOM	336		EU A		21.665	37.524	43.477	1.00 31.72	6
	ATOM	337		EU A		21.954	37.747	42.301	1.00 29.76	6
55	ATOM	338		YS A		21.157	38.439	44.298	1.00 29.33	8
رر	ATOM	_		YS A		20.868	39.800	43.864		7
	ATOM			YS A		20.293	40.615	45.026	1.00 34.28	6
	ATOM	_		YS A		18.919	40.163	45.511	1.00 35.98	6
	ATOM	342	CD L	YS A	306	18.397	41.127		1.00 43.35	6
						- - -	/	30.333	1.00 51.50	6

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5	ATOM	343	CE I	YS A	306				1.00 53.26	
_	ATOM	344	NZ I	YS A	306		-		1.00 59.61	
	ATOM	345	C I	YS A	306	22.075		43.302	1.00 35.25	
	ATOM	346	o I	YS A	306	21.972		42.334	1.00 33.95	
	ATOM	347		SLY A		23.228	40.306	43.928	1.00 35.79	
10	ATOM	348		GLY A		24.445	40.962	43.482	1.00 34.59	
. •	ATOM	349	c (GLY A	307	25.109	40.353	42.259	1.00 33.80	
	ATOM	350	0 (GLY A	307	25.489	41.087	41.344	1.00 31.5	
	ATOM	351	N (CYS A	308	25.248	39.024	42.256	1.00 31.1	
	ATOM	352	CA	CYS A	308	25.899	38.326	41.174	1.00 29.0	
15	ATOM	353	СВ	CYS A	308	26.604	37.089	41.704	1.00 27.5	
13	ATOM	354	SG	CYS A	308	25.472	35.770	42.071	1.00 30.5	
	ATOM	355	С	CYS A	308	24.974	37.870	40.062	1.00 30.5	
	ATOM	356		CYS A		25.458	37.319	39.077	1.00 33.7	
	ATOM	357		CYS A		23.664	38.084	40.195	1.00 28.4	
20	ATOM	358		CYS A		22.739	37.623	39.168	1.00 30.1	
20	ATOM	359		CYS A		21.311	38.004	39.490	1.00 33.4	
	ATOM	360	SG	CYS A	309	20.198	37.299	38.307	1.00 35.2	
	ATOM	361	С	CYS A		23.065	38.123	37.788	1.00 27.7	
	ATOM	362	0	CYS A		23.212	37.334	36.865	1.00 27.6	
25	ATOM	363	N	MET A		23.157	39.439	37.639	1.00 26.1	
23	MOTA	364	CA	MET F		23.476	40.016	36.342	1.00 26.0	
	ATOM	365	CB	MET F		23.482	41.547	36.419	1.00 25.3	
	ATOM	366	CG	MET A	310	23.913	42.230	35.109	1.00 24.0	
	ATOM	367	SD	MET A		22.765	41.751	33.762	1.00 27.	
30	ATOM	368	CE	MET A		23.650	42.321	32.270	1.00 28.5	
50	ATOM	369	С	MET A	A 310	24.842	39.527	35.908	1.00 25.9	
	MOTA	370	0	MET A	A 310	25.020	39.076	34.788	1.00 28.0	
	ATOM	371	N	GLU Z	A 311	25.800	39.638	36.826	1.00 25.3	
	ATOM	372	CA	GLU Z	A 311	27.176	39.234	36.589	1.00 27.0	
35	ATOM	373	CB	GLU 2	A 311	27.973	39.303	37.900	1.00 24.	
	ATOM	374	CG	GLU .	A 311	27.842	40.628	38.668	1.00 26.	
	ATOM	375	CD	GLU .	A 311	28.726	40.720	39.870	1.00 23.	
	MOTA	376	OE1	GLU	A 311	28.891	39.706	40.588	1.00 19.	
	MOTA	377	OE2	GLU	A 311	29.270	41.818	40.159	1.00 26.	
40	ATOM	378	С	GLU	A 311	27.266	37.827	35.997	1.00 27.	
	MOTA	379	0		A 311	27.956	37.620	35.014	1.00 29.	
	MOTA	380	N	ILE	A 312	26.569	36.866	36.602	1.00 26.	
	ATOM	381	CA		A 312	26.593	35.497	36.112	1.00 25. 1.00 23.	
	ATOM	382	CB		A 312	25.991		37.123		
45	MOTA	383			A 312	25.917				
	ATOM	384	CG1		A 312	26.837		38.398		
	MOTA	385	CD1		A 312	26.462				
	MOTA	386	С	ILE	A 312	25.871				
	MOTA	387	0	ILE	A 312	26.274				
50		388	N	MET	A 313	24.788				
•	ATOM	389		MET	A 313	24.013				
	ATOM	390		MET	A 313	22.716				
	ATOM	391		MET	A 313	21.608				
	ATOM	392			A 313	19.892				
55		393			A 313	20.034				
	ATOM	394			A 313	24.834				
	ATOM	395			A 313	25.116				
	ATOM	396			A 314	25.209	37.859	32.253	3 1.00 24	.88 7
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5	ATOM	39	7 CA	SER	A 314	26.00	5 38.472	31.197	1 100 07 00	_
	ATOM	398	в св		A 314					6
	MOTA	399			A 314	26.95				6
	ATOM	400) с		A 314	27.27			_ _	8
	ATOM	40			A 314	27.67				6
10	ATOM	402			A 315					8
	ATOM	403			A 315	27.905				7
	ATOM	404			A 315	29.099				6
	ATOM	405				29.685		=		6
	ATOM	406			A 315	30.675			1.00 20.39	6
15	ATOM	407			A 315	31.866			1.00 18.92	6
15	ATOM				A 315	31.125				6
		408			A 315	28.700		30.597		6
	ATOM	409			A 315	29.304		29 .5 56		8
	ATOM	410			A 316	27.678	34.426			7
20	ATOM	411			A 316	27.151	33.312			6
20	ATOM	412		ARG	A 316	25.915		30.928		
	ATOM	413		ARG	A 316	26.188		32.336		6
	ATOM	414	CD	ARG	A 316	24.934		32.901	- · · · ·	6
	ATOM	415	NE	ARG	A 316	25.245		33.721	1.00 18.78	6
	ATOM	416	CZ		A 316	24.341		34.054	1.00 26.57	7
25	ATOM	417	NH1		A 316	23.084			1.00 30.81	6
	MOTA	418	NH2		A 316	24.701		33.639	1.00 33.71	7
	MOTA	419	С		A 316	26.774		34.776	1.00 33.13	7
	ATOM	420			A 316	26.737		28.794	1.00 28.09	6
	ATOM	421	N		A 317			27.931	1.00 32.41	8
30	ATOM	422	CA		A 317	26.484	34.936	28.571	1.00 28.36	7
	ATOM	423	CB		A 317	26.094		27.264	1.00 26.64	6
	ATOM	424	C		A 317	25.232	36.666	27.418	1.00 22.93	6
	ATOM	425	0		A 317	27.323	35.714	26.417	1.00 28.35	6
	ATOM	426	N			27.398	35.342	25.252	1.00 32.10	8
35	ATOM	427	CA		A 318	28.286	36.396	27.026	1.00 29.12	7
	ATOM	428			A 318	29.515	36.760	26.350	1.00 27.50	6
	ATOM	429	CB		A 318	30.434	37.452	27.333	1.00 28.39	6
	ATOM		C		A 318	30.181	35.502	25.825	1.00 28.10	6
	ATOM	430	0		A 318	30.600	35.447	24.678	1.00 28.18	8
40	ATOM	431	N		A 319	30.255	34.491	26.700	1.00 29.16	7
40		432	CA		A 319	30.880	33.198	26.393	1.00 35.24	6
	ATOM	433	CB		A 319	30.703	32.210	27.547	1.00 27.34	6
	ATOM	434		VAL A		30.895	32.891	28.858	1.00 29.96	6
	ATOM	435		VAL A		29.353	31.552	27.482	1.00 31.70	,6
45	ATOM	436	С	VAL A		30.215	32.608	25.165	1.00 40.01	6
45	ATOM	437	0	VAL A	319	30.640	31.575	24.680	1.00 42.70	
	MOTA	438	N	ARG A	320	29.176	33.284	24.683	1.00 38.64	8
	ATOM	439	CA	ARG A	320	28.415	32.822	23.545		7
	ATOM	440	CB	ARG A		27.031	32.458	24.043	1.00 38.61	6
	ATOM	441	CG	ARG A		26.863	30.991		1.00 37.26	6
50	ATOM	442	CD	ARG A		25.637	30.642	24.192	1.00 43.12	6
	ATOM	443	NE	ARG A		25.258		25.014	1.00 50.79	6
	ATOM	444	CZ	ARG A		24.331	29.256	24.770	1.00 54.71	7
	ATOM	445		ARG A			28.625	25.501	1.00 57.89	6
	ATOM	446		ARG A		23.667	29.291	26.440	1.00 49.08	7
55	ATOM	447		ARG A		23.964	27.385	25.242	1.00 59.59	7
	ATOM	448				28.292	33.825	22.405	1.00 42.14	6
	ATOM	449		ARG A		27.251	33.909	21.748	1.00 46.30	8
	ATOM	450		TYR A		29.352	34.583	22.173	1.00 42.04	7
		300	CA	TYR A	321	29.366	35.555	21.098	1.00 42.70	6

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5	MOTA	451		YR A 32		••••		20.448	1.00 3		6
	MOTA	452		YR A 32		• • • • • •	38.296	19.574	1.00 3		6
	MOTA	453		YR A 32			39.037	18.494	1.00 3		6
	MOTA	454		YR A 32		30.235	37.743	20.224	1.00 2		6
	ATOM	455		YR A 32		31.966	38.475	19.153	1.00 3		6
10	MOTA	456		YR A 32		32.473		18.276	1.00 3		6
	MOTA	457		YR A 32		31.612	39.125	17.223	1.00 3		8
	ATOM	458		YR A 32		32.107	39.866	19.877	1.00 4		6
	MOTA	459		YR A 32		30.085	35.005	19.951	1.00 4		8
	MOTA	460		YR A 32		31.261	34.697		1.00 4		7
15	MOTA	461		ASP A 32		29.354	34.879	18.773	1.00		6
	ATOM	462		ASP A 32		29.912	34.400	17.502	1.00		6
	ATOM	463		ASP A 3		28.804	33.670	16.736	1.00		6
	ATOM	464		ASP A 3		29.050	33.608	15.255	1.00		8
	ATOM	465		ASP A 3		30.010	34.256	14.768			
20	ATOM	466	OD2	ASP A 3	22	28.262	32.929	14.536	1.00		8
	ATOM	467	C i	ASP A 3	22	30.460	35.629	16.755	1.00		6
	ATOM	468	0	ASP A 3	22	29.678	36.464	16.271	1.00		8
	ATOM	469	N	PRO A 3	23	31.800	35.735	16.584	1.00		7
	ATOM	470	CD	PRO A 3	23	32.774	34.719	16.991	1.00		6
25	ATOM	471	CA	PRO A 3	23	32.424	36.889	15.890	1.00		6
23	ATOM	472		PRO A 3	23	33.921	36.603	15.936	1.00		6
	ATOM	473		PRO A 3		34.099	35.303	16.582		43.93	6
	ATOM	474	С	PRO A 3	323	31.953	37.087	14.453		48.34	6
	ATOM	475		PRO A 3		31.797	38.210	13.960		50.84	8
30	ATOM	476		GLU A 3		31.778	35.970	13.752		52.39	7
30	ATOM	477		GLU A 3		31.339	35.968	12.370		55.85	6
	ATOM	478		GLU A 3	324	31.035	34.528	11.965		55.54	6
	ATOM	479		GLU A 3		32.224	33.584	12.104		40.00	6
	ATOM	480		GLU A		33.432	34.023	11.310		40.00	6
35	ATOM	481		GLU A		33.350	35.040	10.555		40.00	8
33	ATOM	482		GLU A		34.506	33.356	11.415		40.00	8
	ATOM	483		GLU A		30.077	36.798	12.277		54.94	6
	ATOM	484		GLU A	324	30.070	37.892	11.730		59.81	8
	ATOM	485		SER A		29.009	36.212	12.810		52.95	7
40	ATOM	486		SER A		27.695	36.812	12.839		50.10	6
40	ATOM	48		SER A		26.701		13.402		48.23	6
	ATOM	488		SER A		27.183	35.239			48.71	8
	ATOM	489		SER A		27.651	38.093			50.61	6
	ATOM	490		SER A		26.885	38.992	13.354		52.19	8
45		49		GLU A		28.495	38.168	14.687		45.64	7
43	ATOM	49		GLU A		28.567		15.546		43.35	6
	ATOM	49		GLU A		28.830		14.711		42.74	6
		49		GLU A		30.148		13.945		50.32	6
	ATOM ATOM	49		GLU A		30.451		13.313		56.34	6
50		49		GLU A		31.509		_		59.31	8
50		49		GLU A		29.656			1.00	55.74	8
	MOTA			GLU A		27.288				40.23	6
	ATOM	49		GLU A		26.695				40.44	8
	MOTA	49		THR A		26.888				35.90	7
=	ATOM	50				25.663				37.29	6
55		. 50		THR A		24.466				37.63	6
	ATOM	50		THR A		24.466				38.12	8
	MOTA	50		THR A		24.269				39.90	
	MOTA	50	14 CG2	2 THR A	321	24.20	30.30	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			

5	ATCM	505	С	THR	Α	327	25.767	37.562	19.038	1.00	39.49	6
	ATOM	506	0			327	26.284	36.458	18.903		40.50	8
	ATOM	507	N			328	25.250	37.987	20.184		36.64	7
	ATOM	508	CA			328	25.264	37.141	21.381		37.73	6
	ATOM	509	ĆB			328	25.148	37.999	22.650		37.78	
10	ATOM	510	CG			328	26.102	39.150	22.843		36.26	6
	ATOM	511		LEU			26.066	39.623	24.272			6
	ATOM	512		LEU			27.481	38.688			36.56	6
	ATOM	513	C			328	24.063	36.220	22.500		39.85	6
	ATOM	514	Ö			328			21.244		37.27	6
15	ATOM	515	N			329	23.306	36.337	20.279		34.96	8
	ATOM	516	CA			329	23.891	35.317	22.205		39.73	7
	ATOM	517	CB				22.785	34.376	22.180		40.81	6
	ATOM	517	OG1			329	23.241	32.991	21.699		42.67	6
	ATOM	519				329	23.879	33.103	20.421		42.52	8
20			CG2				22.026	32.057	21.589		43.52	6
20	ATOM	520	С			329	22.168	34.245	23.548		44.31	6
	ATOM	521	0	THR			22.526	33.370	24.320	1.00	43.72	8
	ATOM	522	N	LEU			21.237	35.149	23.830		44.62	7
	MOTA	523	CA	LEU	-		20.532	35.170	25.111		45.09	6
25	ATOM	524	СВ	LEU			19.677	36.444	25.195	1.00	44.66	6
25	ATOM	525	CG	LEU			20.436	37.750	25.259		51.06	6
	ATOM	526	CD1	LEU			21.405	37.831	24.104	1.00	48.58	6
	ATOM	527		LEU			19.466	38.909	25.238		45.18	6
	MOTA	528	C	LEU			19.656	33.919	25.301		48.06	6
30	ATOM	529	0	LEU			19.049	33.422	24.359		49.33	8
30	ATOM	530	N	ASN			19.618	33.431	26.540		52.20	7
	ATOM	531	CA	ASN			18.842	32.256	26.913		54.41	6
	ATOM	532	CB	ASN			17.361	32.628	27.009		54.94	6
	ATOM ATOM	533	CG	ASN			16.724	32.112	28.269		60.35	6
35		534		ASN			17.124	32.505	29.383		61.84	8
33	ATOM	535	ND2	ASN			15.750	31.238	28.117		65.92	7
	ATOM	536	С	ASN		•	19.016	31.108	25.934	1.00		6
	ATOM ATOM	537 538	0	ASN			18.243	30.157	25.941		60.17	8
	ATOM	539	N	GLY			20.063	31.196	25.114	1.00		7
40	ATOM		CA	GLY			20.341	30.161	24.131		58.55	6
40	ATOM	540	С	GLY			19.316	30.016	23.021		59.79	6
	ATOM	541	0	GLY			19.413	29.094	22.213		61.32	8
	ATOM	542 543	N	GLU			18.346	30.929	22.983		60.28	7
	ATOM	544	CA	GLU			17.294	30.883	21.985		59.13	6
45	ATOM	545	CB	GLU			15.919	30.875	22.662		62.40	6
43	ATOM		CG	GLU			15.667	29.750	23.658		75.69	6
	ATOM	546	CD	GLU			14.341	29.865	24.346		80.41	6
		547		GLU			14.052	30.932	24.945		79.98	8
	ATOM ATOM	548		GLU			13.549	28.884	24.329	1.00	83.81	8
50		549	C	GLU			17.356	32.090	21.073		57.18	6
50	ATOM	550	0	GLU			17.239	31.969	19.852	1.00	57.50	8
	ATOM	551	N	MET			17.512	33.258	21.696	1.00	55.20	7
	ATOM	552	CA	MET			17.561	34.529	20.980	1.00	50.85	6
	ATOM	553	СВ	MET			16.751	35.556	21.763	1.00	48.70	6
55	ATOM	554	CG	MET			16.859	36.947	21.212	1.00	45.39	6
55	ATOM	555	SD	MET			15.881	38.186	22.127	1.00	44.56	16
	ATOM	556	CE	MET			14.229	37.371	22.113		45.25	6
	ATOM	557	С	MET			18.956	35.087	20.713	1.00	51.59	6
	MOTA	558	0	MET	A	334	19.739	35.268	21.633	1.00	52.52	8

5	ATOM	559	N	ALA A	335	19.234	35.371	19.444	1.00 5	1.00	7
	ATOM	560	CA	ALA A	335	20.520	35.932	19.039	1.00 4	8.98	6
	ATOM	561	СВ	ALA A	335	20.997	35.254	17.768	1.00 4	7.86	6
	MOTA	562	С	ALA A	335	20.342	37.420	18.805	1.00 5	1.01	6
	ATOM	563		ALA A		19.594	37.830	17.919	1.00 5	1.61	8
10	ATOM	564	N	VAL A	336	21.024	38.232	19.612	1.00 4	6.62	7
	ATOM	565	CA	VAL A		20.910	39.699	19.502	1.00 4	12.35	6
	ATOM	566	СВ	VAL A		20.517	40.325	20.840	1.00 4	12.41	6
	ATOM	567		VAL A		19.242	39.691	21.361	1.00 4	12.00	6
	ATOM	568		VAL A		21.639	40.211	21.852	1.00 4	10.32	6
15	ATOM	569	С	VAL A		22.204	40.321	19.036	1.00 4	15.33	6
	ATOM	570	0	VAL A		23.263	39.691	19.025	1.00	17.42	8
	ATOM	571	N	THR A		22.090	41.590	18.668	1.00	11.60	7
	ATOM	572	CA	THR A		23.230	42.377	18.175	1.00		6
	ATOM	573	СВ	THR A		22.882	43.061	16.852	1.00		6
20	ATOM	574	OG1	THR A		21.987	44.157	17.080	1.00		8
20	ATOM	575	CG2	THR A		22.216	42.067	15.904	1.00		6
	ATOM	576	C	THR A		23.588	43.481	19.159	1.00		6
	ATOM	577	0	THR A		22.734	43.989	19.892	1.00	34.06	8
	ATOM	578	N	ARG A		24.865	43.849	19.138	1.00		7
25	ATOM	579	CA	ARG A		25.388	44.919	19.984	1.00		6
	ATOM	580	СВ	ARG A		26.669	45.479	19.351	1.00		6
	ATOM	581	CG	ARG A		27.250	46.713	20.038	1.00		6
	ATOM	582	CD	ARG A		28.443	47.254	19.247	1.00		6
	ATOM	583	NE	ARG A		29.559	46.320	19.175	1.00		7
30	ATOM	584	CZ	ARG A		30.449	46.122	20.145	1.00		6
50	ATOM	585	NH1	ARG A		30.338	46.791	21.295	1.00		7
	ATOM	586		ARG A		31.433	45.240	19.954	1.00	27.40	7
	ATOM	587	С	ARG A		24.333	46.010	20.085	1.00		6
	ATOM	588	Ö	ARG A		23.894	46.397	21.169	1.00		8
35	ATOM	589	N	GLY A		23.915	46.496	18.922	1.00		7
22	ATOM	590	CA	GLY A		22.918	47.547	18.890	1.00		6
	ATOM	591	C	GLY A		21.692	47.140	19.672	1.00		6
	ATOM	592	0	GLY A		21.445	47.671	20.750	1.00	38.30	8
	ATOM	593	N	GLN A		20.924	46.203	19.105	1.00	38.58	7
40	ATOM	594	CA	GLN A		19.701	45.700	19.729		40.79	6
••	ATOM	595	CB	GLN A		19.436	44.260	19.253	1.00	40.82	6
	ATOM	596	CG	GLN A		19.087	44.146	17.767	1.00	41.10	6
	ATOM	597	CD	GLN A		18.876	42.705	17.305		48.84	6
	ATOM	598		GLN A		19.826	41.888	17.309	1.00	50.53	8
45	ATOM	599				17.650	42.393	16.907		54.25	7
,,,	ATOM	600	С	GLN A		19.779	45.750	21.263	1.00	41.50	6
	ATOM	601	Ō	GLN A		18.998	46.444	21.923		42.72	8
	ATOM	602	N	LEU P		20.758	45.026	21.806		42.00	7
	ATOM	603	CA	LEU P		20.952	44.947	23.243		38.10	6
50	ATOM	604	СВ	LEU F		22.209	44.145	23.575		36.66	6
50	ATOM	605	CG	LEU F		22.361	43.804	25.029		39.94	6
	ATOM	606		LEU F		21.219	42.884	25.410		34.98	6
	ATOM	607		LEU A		23.685	43.128	25.284		40.95	6
	ATOM	608	C	LEU F		21.072	46.321	23.860		36.37	6
55	ATOM	609	0	LEU F		20.484	46.588	24.892		37.89	8
دد		610	N	LYS F		21.848	47.184	23.209		33.29	7
	ATOM					22.089	48.546	23.679		35.17	6
	ATOM	611	CA	LYS				22.721		34.97	6
	ATOM	612	СВ	LYS A	342	23.057	49.242	66.161	1.00	33.31	U

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5	ATOM	613	CG			342	23.655	50.536	23.240	1.00 40.00	6
	ATOM	614	CD			342	24.673	51.109	22.245	1.00 34.48	6
	MOTA	615	CE			342	25.514	52.229	22.873	1.00 37.54	6
	ATOM	616	NZ			342	26.655	52.634	21.987	1.00 42.32	7
10	ATOM ATOM	617	С			342	20.796	49.349	23.774	1.00 38.29	8
10	ATOM	618	0			342	20.345	49.711	24.861	1.00 36.23	8
	ATOM	619 620	N			343	20.223	49.622	22.603	1.00 39.25	7
	ATOM	621	CA			343	18.993	50.385	22.485	1.00 40.19	6
			CB			343	18.521	50.373	21.033	1.00 37.96	6
15	ATOM ATOM	622	CG			343	19.664	50.550	20.052	1.00 39.22	6
13	ATOM	623 624		ASN			20.428	51.537	20.125	1.00 42.37	8
	ATOM	625	ND2				19.773	49.612	19.125	1.00 42.19	7
	ATOM	626	С			343	17.928	49.748	23.375	1.00 40.12	6
	ATOM	627	0	ASN			17.010	50.417	23.859	1.00 36.01	8
20	ATOM	628	N	GLY			18.073	48.433	23.568	1.00 40.95	7
20	ATOM	629	CA C	GLY			17.152	47.670	24.394	1.00 39.25	6
	ATOM	630	0	GLY			17.039	48.092	25.842	1.00 38.26	6
	ATOM	631	N	GLY		•	16.072	47.724	26.512	1.00 35.69	8
	ATOM	632	CA	GLY GLY			18.017	48.857	26.329	1.00 35.89	7
25	ATOM	633	C	GLY			17.964	49.301	27.706	1.00 34.00	6
	ATOM	634	0	GLY			19.273 19.469	49.199	28.443	1.00 38.64	6
	ATOM	635	N	LEU			20.170	49.888	29.441	1.00 38.14	8
	ATOM	636	CA	LEU				48.337	27.973	1.00 39.52	7
	ATOM	637	CB	LEU			21.444 22.124	48.180	28.649	1.00 36.05	6
30	ATOM	638	CG	LEU			21.355	46.876 45.617	28.209	1.00 35.72	6
	ATOM	639	CD1				22.295	44.413	28.501 28.422	1.00 34.89	6
	ATOM	640		LEU			20.786	45.721	29.902	1.00 44.09 1.00 34.84	6
	MOTA	641	С	LEU	•		22.358	49.361	28.396	1.00 34.84	6 6
	ATOM	642	0	LEU			23.267	49.653	29.178	1.00 35.52	8
35	ATOM	643	N	GLY			22.087	50.056	27.295	1.00 30.47	7
	MOTA	644	CA	GLY	Α	347	22.909	51.192	26.931	1.00 33.01	6
	MOTA	645	С	GLY	A	347	24.360	50.768	26.747	1.00 30.72	6
	ATOM	646	0	GLY	Α	347	24.669	49.775	26.082	1.00 30.89	8
	MOTA	647	N	VAL	A	348	25.244	51.556	27.355	1.00 31.30	7
40	ATOM	648	CA	VAL	A	348	26.671	51.325	27.286	1.00 31.27	6
	ATOM	649	СВ	VAL	Α	348	27.441	52.294	28.184	1.00 31.66	6
	ATOM	650		VAL			27.067	52.107	29.631	1.00 20.19	6
	MOTA	651	CG2	VAL			28.931	52.138	27.986	1.00 24.77	6
	ATOM	652	С	VAL			27.063	49.892	27.678	1.00 33.84	6
45	MOTA	653	0	VAL			28.095	49.392	27.225	1.00 29.99	8
	ATOM	654	N	VAL			26.253	49.227	28.514	1.00 33.31	7
	MOTA	655	CA	VAL			26.568	47.881	28.906	1.00 32.23	6
	ATOM	656	CB	VAL .			25.581	47.259	29.858	1.00 32.59	6
50	ATOM	657		VAL .			25.865	45.795	29.985	1.00 33.68	6
50	ATOM	658		VAL .			25.687	47.899	31.213	1.00 32.30	6
	ATOM	659	С	VAL .			26.706	46.985	27.726	1.00 34.91	6
	ATOM	660	0	VAL .			27.583	46.136	27.735	1.00 33.73	8
	ATOM	661	N	SER			25.875	47.134	26.702	1.00 32.81	7
£	ATOM	662	CA	SER A			26.001	46.252	25.556	1.00 30.10	6
55	ATOM	663	СВ	SER A			25.119	46.665	24.411	1.00 24.95	6
	ATOM	664	OG	SER I			25.209	45.675	23.394	1.00 23.16	8
	ATOM	665	С	SER A			27.445	46.257	25.129	1.00 31.59	6
	ATOM	666	0	SER I	4	350	28.116	45.244	25.284	1.00 37.62	8

_					252	27.945	47.367	24.591	1.00 28.60	7
5	MOTA	-		ASP A		29.351	-	24.183	1.00 29.82	6
	ATOM			ASP A		29.808	48.891	24.105	1.00 27.49	6
	ATOM			ASP A		28.875	49.744	23.303	1.00 30.22	6
	ATOM			ASP A		28.055	50.483	23.909	1.00 32.61	8
	MOTA	671		ASP A		28.942	49.714	22.044	1.00 30.02	8
10	MOTA	672		ASP A			46.653	25.231	1.00 30.63	6
	MOTA	673		ASP A		30.173	45.792	24.903	1.00 29.54	8
	MOTA	674		ASP A		30.981	46.949	26.503	1.00 25.33	7
	MOTA	675		ALA A		29.939	46.280	27.602	1.00 28.59	6
	MOTA	676		ALA A		30.623	46.799	28.922	1.00 20.95	6
15	MOTA	677	CB	ALA A		30.072	44.756	27.527	1.00 29.69	6
	MOTA	678	С	ALA A		30.492		27.527	1.00 30.36	8
	MOTA	679	0	ALA A		31.481	44.054	27.387	1.00 27.63	7
	ATOM	680	N	ILE A		29.260	44.260	27.413	1.00 27.55	6
	MOTA	681	CA	ILE A		29.003	42.832		1.00 27.33	6
20	MOTA	682	CB	ILE A		27.512	42.528	27.429	1.00 28.04	6
	MOTA	683	CG2	ILE A		27.269	41.042	27.289	1.00 23.88	6
	MOTA	684	CG1	ILE A		26.955	42.965	28.789	1.00 27.33	6
	ATOM	685	CD1	ILE A		25.452	42.688	28.944	1.00 26.23	6
	MOTA	686	С	ILE P		29.534	42.207	26.054	1.00 30.88	8
25	ATOM	687	0	ILE F		30.007	41.076	26.068		7
	ATOM	688	N	PHE F		29.426	42.917	24.939	1.00 29.86	6
	MOTA	689	CA	PHE A		29.922	42.369	23.686	1.00 31.08	6
	MOTA	690	CB	PHE A		29.371	43.146	22.487	1.00 28.80	6
	ATOM	691	CG	PHE A		28.029	42.643	21.988	1.00 28.80	
30	MOTA	692	CD1			26.872	42.842	22.724	1.00 30.96	6 6
	MOTA	693	CD2			27.950	41.953	20.783	1.00 29.45	6
	ATOM	694	CE1	PHE A	A 354	25.657	42.360	22.250	1.00 27.12	6
	ATOM	695	CE2		A 354	26.738	41.470	20.305	1.00 25.19	6
	MOTA	696	CZ		A 354	25.590	41.672	21.038	1.00 28.09 1.00 29.17	6
35	MOTA	697	С		A 354	31.444	42.399	23.682		8
	MOTA	698	0		A 354	32.087	41.389	23.398	1.00 32.62	7
	ATOM	699	N		A 355	32.013	43.569	23.980	1.00 23.86	6
	ATOM	700	CA		A 355	33.466	43.739	24.030	1.00 25.34 1.00 21.41	6
	MOTA	701	CB		A 355	33.820	45.053	24.737		6
40	MOTA	702	ÇG		A 355	33.841	46.226	23.809	1.00 32.08	8
	ATOM	703		L ASP		32.979	46.322	22.902	1.00 33.58	8
	MOTA	704	OD2	2 ASP	A 355	34.711			1.00 33.20	_
	ATOM	705	С		A 355	34.074	42.559	24.781		6
	MOTA	706	0		A 355	35.131	42.053			8 7
45	MOTA	707	N	LEU	A 356	33.387				
	ATOM	708	CA	LEU	A 356	33.845				6
	ATOM	709	CB	LEU	A 356	32.893				6
	ATOM	710	CG	LEU	A 356	33.235			_	6
	ATOM	711		1 LEU	A 356	34.538				6
50		712			A 356	32.149	39.414			6
•	ATOM	713			A 356	33.849	39.779			6
	MOTA	714			A 356	34.884				8
	ATOM	715			A 357	32.661	39.451			7
	ATOM	716			A 357	32.511				6
55		717			A 357	33.653				6
,,	MOTA	718			A 357	34.302				
	MOTA	719			A 358	33.876		22.564	1 1.00 33.31	
	ATOM	720			A 358	34.949		21.580	1.00 35.87	6
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5	ATOM	721	СВ	MET A	358	35.143	40.606	21.009	1.00 34.56	6
	ATOM	722	CG	MET A	358	33.949	41.145	20.290	1.00 46.43	6
	MOTA	723	SD	MET A	358	34.207	42.776	19.514	1.00 42.13	16
	MOTA	724	CE	MET A	358	34.507	43.855	20.994	1.00 44.29	6
	ATOM	725	С	MET A	358	36.256	38.762	22.230	1.00 33.26	6
10	ATOM	726	0	MET A	358	36.894	37.807	21.795	1.00 36.39	8
	ATOM	727		SER A		36.637	39.491	23.281	1.00 33.31	7
	ATOM	728		SER A		37.860	39.226	24.019	1.00 34.39	6
	ATOM	729		SER A		37.869	40.067	25.295	1.00 30.84	6
	ATOM	730		SER A		39.135	40.008	25.930	1.00 47.14	8
15	ATOM	731	C	SER A		37.984	37.748	24.357	1.00 36.43	6
13	ATOM	732	0	SER A		38.900	37.078	23.896	1.00 35.46	8
	ATOM	733		LEU A		37.046	37.264	25.166	1.00 36.74	7
	MOTA	734		LEU A		37.017	35.875	25.604	1.00 35.44	6
	ATOM	735	CB	LEU A		35.708	35.579	26.336	1.00 34.16	6
20	ATOM	736	CG	LEU A		35.471	36.290	27.644	1.00 34.59	6
20	ATOM	737		LEU A		34.225	35.765	28.312	1.00 33.53	6
		737				36.658	36.052	28.541	1.00 31.69	6
	ATOM	739	C	LEU A		37.203	34.862	24.500	1.00 38.72	6
	MOTA	740	0	LEU A		37.820	33.828	24.728	1.00 38.29	8
25	ATOM ATOM	741	N	SER A		36.635	35.147	23.328	1.00 40.96	7
23		741	CA	SER A		36.777	34.262	22.186	1.00 45.67	6
	ATOM ATOM	743	CB	SER F		36.518	35.045	20.904	1.00 46.45	6
	ATOM	744	OG	SER F		35.210	35.598	20.906	1.00 51.81	8
	ATOM	745	C	SER F		38.166	33.627	22.145	1.00 44.49	6
30	ATOM	746	0	SER F		38.347	32.538	21.625	1.00 46.67	8
30	ATOM	747	N	SER A		39.134	34.348	22.703	1.00 41.44	7
	ATOM	748	CA	SER A		40.525	33.918	22.790	1.00 42.13	6
	MOTA	749	CB	SER A		41.408	35.131	23.066	1.00 42.61	6
	ATOM	750	OG	SER A		41.219	36.136	22.076	1.00 51.87	
35	ATOM	751	С	SER A		40.798	32.870	23.876	1.00 38.41	6
55	ATOM	752	0	SER A		41.553	31.938	23.641	1.00 38.01	
	ATOM	753	N	PHE A		40.198	33.039	25.058	1.00 34.55	
	ATOM	754	CA	PHE A		40.417	32.126	26.174	1.00 32.96	
	ATOM	755	CB	PHE A		39.832	32.718	27.447	1.00 31.99	
40	ATOM	756	CG		363	40.448	34.036	27.840	1.00 29.97	
	ATOM	757		PHE A		40.102	34.650	29.020	1.00 30.61	
	ATOM	758		PHE A		41.379	34.646	27.014	1.00 32.02	6
	ATOM	759		PHE A		40.685	35.856	29.391	1.00 33.67	
	ATOM	760		PHE 2		41.959	35.843	27.377	1.00 30.91	
45	ATOM	761	CZ		363	41.615	36.456	28.558	1.00 29.33	
73	ATOM	762	C		A 363	39.883	30.716	25.967	1.00 30.52	
	ATOM	763	0		A 363	40.436	29.766	26.526	1.00 32.19	
	ATOM	764	N		A 364	38.817	30.570	25.175	1.00 33.51	
	ATOM	765	CA		A 364	38.239	29.264	24.918	1.00 38.03	
50	ATOM	766	CB		A 364	39.240	28.404	24.139	1.00 42.32	
30		767	CG		A 364	39.696	29.065	22.861	1.00 53.11	
	ATOM			ASN A		38.874	29.330	21.954	1.00 59.51	
	ATOM	768					29.330	22.772	1.00 55.95	
	ATOM	769		ASN A		40.986	29.330	26.235	1.00 33.93	
. .	ATOM	770	С		A 364	37.916		26.233	1.00 31.89	
55	ATOM	771	0		A 364	38.324	27.428	27.094	1.00 30.20	
	ATOM	772	N		A 365	37.176	29.271	28.406	1.00 27.82	
	ATOM	773	CA		A 365		28.743		1.00 29.36	
	ATOM	774	СВ	LEU .	A 365	36.195	29.866	29.237	1.00 27.54	. 0

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5	ATOM	775	CG	LEU	Α	365	36.	. 990	31.15	0 2	9.185	1.00	38.91	6
	ATOM	776	CD1	LEU	Α	365	36.	316	32.21	6 3	0.036	1.00	34.47	6
	ATOM	777	CD2	LEU	Α	365	38.	406	30.88	3 2	9.663	1.00	34.24	6
	ATOM	778	С	LEU		365	35.	.830	27.59		8.262		26.23	6
	ATOM	779	0	LEU				890	27.64		7.472		27.06	8
10	ATOM	780	N	ASP				.083	26.52		9.021		25.23	7
	ATOM	781	CA	ASP				.213	25.35		8.988		26.07	6
	ATOM	782	СВ	ASP				.027	24.04		9.033		29.68	6
	ATOM	783	CG	ASP				.799	23.87		0.303		35.74	6
	ATOM	784		ASP				.285	24.17		1.402		36.78	8
15	ATOM	785	OD2	ASP				.959	23.38		0.240		41.23	8
	ATOM	786	C	ASP				.278	25.43		0.181		27.70	6
	ATOM	787	0	ASP				.587	26.09		1.173		31.94	8
	ATOM	788	N	ASP				.141	24.74		0.066		29.18	7
	ATOM	789	CA	ASP				.120	24.67		1.120		32.72	6
20	ATOM	790	СВ	ASP				.472	23.28		1.147		38.04	6
	ATOM	791	CG	ASP				.806	22.92		9.854		42.43	6
	ATOM	792		ASP				.877	23.65		9.409		35.95	8
	ATOM	793	OD2	ASP				.186	21.88		9.250	1.00		8
	ATOM	794	C	ASP				.754	24.96		2.482		33.71	6
25	ATOM	795	0	ASP				.484	26.00		3.098		38.30	8
20	ATOM	796	N	THR				.602	24.03		2.919		31.06	7
	ATOM	797	CA	THR				.329	24.12		4.181		26.28	6
	ATOM	798	CB	THR				.559	23.22		4.141		27.30	6
	ATOM	799	OG1	THR				.161	21.87		3.885		33.42	8
30	ATOM	800	CG.2	THR				.323	23.30		5.454		25.16	6
50	ATOM	801	C	THR				.764	25.55		4.479		21.13	6
	ATOM	802	0	THR				.408	26.15		5.503		23.17	8
	ATOM	803	N	GLU	•	•		.545	26.09		3.551		21.32	7
	ATOM	804	CA	GLU				.065	27.43		3.661		28.00	6
35	ATOM	805	CB	GLU				.960	27.70		2.453		32.79	6
22	ATOM	806	CG	GLU				.089	26.66		2.346		36.29	6
	ATOM	807	CD	GLU				.906	26.74		1.110		41.03	6
	ATOM	808	OE1	GLU				.337	26.74		9.994		42.05	8
	ATOM	809		GLU				.158	26.79		1.218		42.03	8
40	ATOM	810	C	GLU				.953	28.47		3.821		25.57	6
	ATOM	811	Ö	GLU				.987	29.25		4.760		20.56	8
	ATOM		N	VAL				.967	28.46		2.921		25.39	7
	ATOM	813	CA	VAL				.849	29.39		3.029		25.99	6
	ATOM	814	CB	VAL				.763	29.13		1.987		26.15	6
45	ATOM	815		VAL				.609	30.09		2.183		27.65	6
	ATOM	816		VAL				.306	29.25		0.592		17.70	6
	ATOM	817	C	VAL				.245	29.20		4.412		26.49	6
	ATOM	818	0	VAL				.012	30.17		5.147		28.16	
	ATOM	819	N	ALA				.988	27.94				21.01	8 7
50	ATOM	820	CA	ALA					27.55		4.739			
50	ATOM	821	CB					.393			6.011		19.57	6
		822		ALA ALA				.441	26.03		6.145		18.62	6
	ATOM		С					.116	28.21		7.177		23.48	6
	ATOM	823	0	ALA				.531	28.98		7.931		32.67	8
55	ATOM	824	N	LEU				.401	27.89		7.305		22.89	7
55	ATOM	825	CA	LEU				.217	28.44		8.369		23.28	6
	ATOM	826	CB	LEU				.675	27.99		8.178		27.76	6
	ATOM	827	CG	LEU				.943	26.52		8.415		21.18	6
	ATOM	828	CDI	LEU	A	312	37	.356	26.17	1 3	8.049	1.00	27.64	6

5	MOTA	829	CD2	LEU	A	372	35.675	26.204	39.880	1.00 20.90	6
	ATOM	830	С			372	34.098	29.966	38.396	1.00 20.30	
	ATOM	831	0			372	33.828	30.572	39.439	1.00 21.34	
	ATOM	832	N			373	34.288	30.561	37.223	1.00 23.16	
	ATOM	833	CA			373	34.214	32.007	37.223		
10	ATOM	834	СВ			373	34.296	32.360	35.575	1.00 23.78	
	ATOM	835	CG			373	34.784	33.726		1.00 22.18	
	ATOM	836				373	36.000	34.084	35.165	1.00 31.52	
	ATOM	837				373	35.103	33.720	35.962	1.00 31.93	
	ATOM	838	C			373	32.904		33.693	1.00 30.24	
15	ATOM	839	Ö			373	32.895	32.480	37.720	1.00 25.69	
	ATOM	840	N			374	31.814	33.410	38.532	1.00 30.13	
	ATOM	841	CA			374		31.800	37.368	1.00 26.24	7
	ATOM	842	CB			374	30.487	32.104	37.896	1.00 21.60	
	ATOM	843	CG			374	29.454	31.121	37.335	1.00 24.57	6
20	ATOM	844	CD				29.310	31.145	35.821	1.00 21.02	6
	ATOM	845	OE1			374	28.224	30.201	35.331	1.00 22.86	6
	ATOM	846	NE2			374 374	28.037	30.042	34.123	1.00 24.07	8
	ATOM	847	C				27.515	29.590	36.249	1.00 25.59	7
	ATOM	848	0			374	30.421	32.039	39.422	1.00 20.66	6
25	ATOM	849	N			374	29.717	32.832	40.048	1.00 24.47	8
23	ATOM	850				375	31.136	31.074	40.004	1.00 16.26	7
	ATOM	851	CA CB			375	31.155	30.889	41.445	1.00 17.16	6
	ATOM	852	C			375	31.805	29.568	41.780	1.00 19.53	6
	ATOM	853	0			375	31.907	32.025	42.108	1.00 25.13	6
30	ATOM	854	N			375	31.397	32.646	43.034	1.00 23.81	8
50	ATOM	855	CA			376 376	33.122	32.277	41.611	1.00 24.57	7
	ATOM	856	CB			376	33.959	33.354	42.118	1.00 25.80	6
	ATOM	857	CG1			376	35.101	33.658	41.164	1.00 26.48	6
	ATOM	858	CG2			376	35.926	34.812	41.697	1.00 23.20	6
35	ATOM	859	C			376	35.959 33.107	32.429	40.952	1.00 19.08	6
	ATOM	860	0			376	33.297	34.599	42.312	1.00 25.69	6
	ATOM	861	N			377	32.159	35.364	43.251	1.00 27.87	8
	ATOM	862	CA			377	31.242	34.781	41.399	1.00 23.09	7
	ATOM	863	СВ			377	30.540	35.915 36.031	41.423	1.00 22.86	6
40	ATOM	864	CG			377	31.424	36.368	40.061	1.00 18.50	6
	ATOM	865	CD1				30.689	36.227	38.885	1.00 22.65	6
	ATOM	866		LEU			31.916		37.601	1.00 16.70	6
	ATOM	867	C			377	30.228	37.776 35.719	39.051	1.00 19.58	6
	ATOM	868	0	LEU			30.228	36.532	42.543	1.00 26.14	6
45	ATOM	869	N	LEU			29.483	34.614	43.452	1.00 20.62	8
	MOTA	870	CA	LEU			28.469	34.303	42.468	1.00 28.99	7
	ATOM	871	СВ	LEU			28.053		43.475	1.00 28.87	6
	ATOM	872	CG	LEU				32.826	43.397	1.00 26.89	6
	ATOM	873		LEU			27.110	32.344	44.472	1.00 28.83	6
50	ATOM	874		LEU			25.915	33.252	44.525	1.00 27.97	6
	ATOM	875	C	LEU			26.693	30.928	44.205	1.00 27.69	6
	ATOM	876	0	LEU			28.992	34.617	44.853	1.00 31.09	6
	ATOM	877	N	MET			28.399	35.421	45.573	1.00 31.77	8
	ATOM	878	CA	MET			30.118	33.991	45.189	1.00 31.44	7
55	ATOM	879	CB	MET			30.736	34.141	46.494	1.00 32.62	6
	ATOM	880	CG	MET			31.690	32.960	46.744	1.00 31.45	6
	ATOM	881	SD	MET			30.984	31.595	46.792	1.00 38.75	6
	ATOM	882	CE	MET			29.741	31.626	48.107	1.00 41.27	16
	0.1	304	CL	CIEI	A	319	28.896	30.036	47.851	1.00 35.68	6

	5	ATOM	883	С	MET	A	379		35.448	46.727		33.72	6
		MOTA	884	0	MET	Α	379	32.567	35.450	47.305		36.29	8
		ATOM	885	N	SER	A	380	30.889	36.555	46.315	1.00	34.49	7
		ATOM	886	CA	SER	Α	380	31.498	37.853	46.550	1.00	33.97	6
		ATOM	887	CB	SER	Α	380	30.921	38.890	45.576	1.00	31.24	6
	10	ATOM	888	OG	SER	Α	380	31.205	38.543	44.230	1.00	39.42	8
		ATOM	889	С	SER	Α	380	31.179	38.239	47.992	1.00	39.69	6
		ATOM	890	0	SER	Α	380	30.029	38.446	48.357	1.00	44.64	8
		ATOM	891	N	SER	A	381	32.214	38.313	48.812	1.00	41.04	7
		ATOM	892	CA	SER			32.060	38.640	50.216	1.00	44.91	6
	15	ATOM	893	CB	SER			33.324	38.234	50.951	1.00	44.50	6
		ATOM	894	OG	SER			34.431	39.002	50.510	1.00	45.42	8
•		ATOM	895	С	SER			31.795	40.106	50.499	1.00	44.59	6
		ATOM	896	0	SER			31.476	40.470	51.618		49.32	8
		ATOM	897	N	ASP			31.939	40.942	49.486		43.75	7
	20	ATOM	898	CA	ASP			31.744	42.362	49.641		43.93	6
	20	ATOM	899	СВ	ASP			32.673	43.111	48.677		48.39	6
		ATOM	900	CG	ASP			32.572	42.624	47.263		53.23	6
		ATOM	901		ASP			32.705	41.400	47.034		56.97	8
		ATOM	902		ASP			32.358	43.454	46.333		58.91	8
	25	MOTA	903	C	ASP			30.314	42.885	49.507		41.09	6
	23	ATOM	904	0	ASP			30.048	44.036	49.845		40.93	8
		ATOM	905	N	ARG			29.397	42.049	49.034		42.63	7
		ATOM	906	CA	ARG		-	28.036	42.485	48.876		43.32	6
		ATOM	907	CB	ARG			27.138	41.332	48.443		42.31	6
	30	ATOM	908	CG	ARG			27.651	40.399	47.352		40.83	6
	30		909	CD	ARG			27.586	40.954	45.925		38.09	6
		ATOM	910	NE	ARG			27.768	39.878	44.975		37.33	7
		ATOM ATOM	911	CZ	ARG	•		28.037	40.058	43.693		38.35	6
			912		ARG	•	.,	28.142	41.292	43.198		33.70	7
	35	ATOM	913		ARG			28.194	38.992	42.918		35.46	7
	33	ATOM		C	ARG			27.523	42.989	50.216		44.96	6
		ATOM	914 915	0	ARG			27.744	42.344	51.260		45.60	8
		ATOM			PRO		•	26.852	44.144	50.223		45.33	7
		ATOM	916 917	N CD	PRO			26.625	44.964	49.027		46.85	6
	40	ATOM			PRO			26.298	44.738	51.446		47.37	6
	40	ATOM	918	CA						51.446		46.90	6
	•	ATOM	919	CB	PRO			25.841	46.130			_	_
		MOTA	920	CG	PRO			26.075	46.229	49.567 52.049		46.41 48.29	6 6
		ATOM	921	С	PRO			25.158	43.919			48.34	8
	45	ATOM	922	0			384	24.404	43.264	51.329		49.88	7
	45	ATOM	923	N			385	25.039	43.983	53.383			6
		ATOM	924	CA			385	23.991	43.270	54.113		50.35	
		ATOM	925	С			385	24.347	41.852	54.495		50.70	6
		ATOM	926	0			385	23.614	41.204	55.244		53.48	8
		ATOM	927	N			386	25.466	41.371	53.955		49.04	7
	50	ATOM	928	CA			386	25.901	40.017	54.215		50.53	6
		ATOM	929	CB			386	27.224	39.751	53.492		45.17	6
		ATOM	930	CG			386	27.152	39.592	51.993		48.26	6
		ATOM	931		LEU			28.542	39.439	51.404		41.68	6
		MOTA	932		LEU			26.302	38.374	51.682		38.40	6
	55	MOTA	933	С			386	26.045	39.776	55.691		52.13	6
		ATOM	934	0			386	26.296	40.692	56.459		53.67	8
		ATOM	935	N			387	25.861	38.522	56.077		53.42	7
		ATOM	936	CA	ALA	A	387	25.976	38.129	57.470	1.00	56.01	6

5	ATOM	937	СВ	ALA	A	387	24.802	37	.234	57.854	1.00	56.47	6
	MOTA	938	С	ALA	A	387	27.289	37	.385	57.659	1.00	55.52	6
	ATOM	939	0	ALA	Α	387	28.275	37	.940	58.134	1.00	53.75	8
	ATOM	940	N	CYS	А	388	27.273	36	.120	57.253	1.00	56.03	7
	ATOM	941	CA	CYS	Α	388	28.412	35	.236	57.370	1.00	59.57	6
10	ATOM	942	CB	CYS	Α	388	27.923	33	.803	57.172	1.00	59.23	6
	ATOM	943	SG	CYS	Α	388	26.397	33	.431	58.009	1.00	58.64	16
	ATOM	944	С	CYS	Α	388	29.482	35	.581	56.328	1.00	62.18	6
	ATOM	945	0	CYS	Α	388	29.720	34	.821	55.400	1.00	67.88	8
	ATOM	946	N	VAL	Α	389	30.110		.747	56.495		60.78	7
15	ATOM	947	CA	VAL			31.173		.212	55.590		57.70	6
	ATOM	948	СВ	VAL			31.740		.567	56.024		57.09	6
	ATOM	949	CG1				32.795		.037	55.041		59.03	6
	ATOM	950	CG2	VAL			30.640		.598	56.171		53.98	6
	ATOM	951	С	VAL			32.297		.182	55.550		57.77	6
20	ATOM	952	0	VAL			32.358		.336	54.662		60.94	8
	ATOM	953	N	ALA			33.182		.292	56.528		52.68	7
	ATOM	954	CA	ALA		•	34.347		.431	56.684		48.41	6
	ATOM	955	CB	ALA			34.703		.321	58.185		45.19	6
	ATOM	956	C	ALA			34.224		.040	56.082		47.63	6
25	ATOM	957	Ö	ALA			35.107		.597	55.348	1.00		8
	ATOM	958	N	ARG		391	33.117		.366	56.391		47.11	7
	ATOM	959	CA	ARG		391	32.879		.018	55.885		51.64	6
	ATOM	960	CB	ARG		391	31.520		.498	56.383		54.22	6
	ATOM	961	CG	ARG		391	31.267		.012	56.059		64.20	6
30	ATOM	962	CD	ARG		391	29.930		.489	56.602		73.80	6
50	ATOM	963	NE	ARG		391	29.787		.044	56.454		79.76	7
	ATOM	964	CZ	ARG			30.573		.140	57.043		84.27	6
	ATOM	965		ARG		•	31.598		.535	57.806		85.28	7
	ATOM	966	NH2				30.340		.840	56.849		86.84	7
35	ATOM	967	C			391	32.922		.986	54.358		48.18	6
3.2	ATOM	968	0			391	33.494		.080	53.756		49.57	8
	ATOM	969	N			392	32.281		.993	53.762		45.01	7
	ATOM	970	CA			392	32.196		.148	52.319		48.77	6
	ATOM	971	CB			392	31.224		.297	51.963		46.45	6
40	ATOM	972	CG2			392	31.241		.582	50.479		42.35	6
• • •	ATOM	973		ILE			29.791		.953	52.402		49.69	6
	ATOM	974		ILE			28.792		.039	52.113		51.09	6
	ATOM	975	C			392	33.554		.356	51.641		50.90	6
	ATOM	976	Ö			392	33.914		.605	50.732		52.21	8
45	ATOM	977	N			393	34.298		.374	52.071		50.43	7
	ATOM	978	CA			393	35.592		.684	51.471		50.30	6
	ATOM	979	CB			393	36.437		.561	52.387		53.97	6
	ATOM	980	CG			393	36.558		.966	51.844		62.18	6
	MOTA	981	CD			393	37.546		.777	52.564		67.69	
50	ATOM	982		GLU			38.149		.741				6
50	ATOM	983		GLU						52.119		66.42	8
							37.856		.640	53.729		70.64	8
	ATOM	984	C			393	36.341		.429	51.230		49.31	6
	ATOM	985	0			393	36.755		.089	50.125		49.53	8
55	ATOM	986	N			394	36.552		.730	52.303		46.07	7
55	ATOM	987	CA			394	37.265		.543	52.078		45.76	6
	ATOM	988	CB			394	37.396		.800	53.373		43.85	6
	ATOM	989	CG			394	38.207		.617	54.394		40.00	6
	MOTA	990	CD	LYS	Α	394	39.372	32	.374	53.705	1.00	40.00	6

5	ATOM	991	CE	LYS	А	394	40.136	33.265	54.681	1.00 40.00	6
	MOTA	992	NZ	LYS	A	394	41.516	33.602	54.162	1.00 40.00	7
	ATOM	993	С	LYS	A	394	36.568	30.778	50.966	1.00 46.69	6
	MOTA	994	0	LYS	Α	394	37.215	30.427	49.988	1.00 49.13	8
	ATOM	995	N	TYR	Α	395	35.269	30.514	51.095	1.00 46.57	
10	ATOM	996	CA	TYR	Α	395	34.553	29.823	50.022	1.00 43.33	6
	MOTA	997	СВ	TYR	Α	395	33.059	30.123	50.076	1.00 48.44	6
	MOTA	998	CG	TYR	Α	395	32.275	29.236	50.994	1.00 53.83	
	ATOM	999	CD1	TYR	Α	395	31.010	29.598	51.415	1.00 56.43	
	ATOM	1000	CE1	TYR			30.266	28.769	52.252	1.00 59.73	
15	ATOM	1001	CD2	TYR			32.790	28.033	51.428	1.00 56.47	
	ATOM	1002	CE2	TYR			32.054	27.198	52.265	1.00.62.60	
	MOTA	1003	CZ			395	30.787	27.565	52.687	1.00 63.18	
	ATOM	1004	ОН			395	30.059	26.753	53.528	1.00 64.46	
	ATOM	1005	С			395	35.120	30.356	48.716	1.00 37.30	
20	ATOM	1006	Ö			395	35.643	29.601	47.908	1.00 37.30	
	ATOM	1007	N			396	35.029	31.670	48.522	1.00 34.10	
	ATOM	1008	CA			396	35.563	32.273	47.305	1.00 31.92	6
	ATOM	1009	CB	GLN		396	35.403	33.801	47.329		
	ATOM	1010	CG	GLN		396	36.088	34.485	46.162	1.00 32.64	6
25	ATOM	1011	CD	GLN		396	35.616	35.891	45.927	1.00 29.57	6
	ATOM	1012	OE1			396	35.599	36.726		1.00 29.46	
	ATOM	1013	NE2			396	35.245	36.173	46.862	1.00 34.65	
	ATOM	1013	C			396	37.035	31.909	44.689	1.00 27.21	7
	MOTA	1015	0	GLN		396	37.511	31.590	47.167	1.00 37.13	
30	ATOM	1016	N	ASP		397	37.751		46.080	1.00 37.36	
50	ATOM	1017	CA	ASP		-	39.164	31.970 31.642	48.285 48.298	1.00 38.61	7
	ATOM	1018	CB	ASP			39.757			1.00 40.37	6
	ATOM	1019	CG	ASP			39.737	31.869	49.704	1.00 40.51	6
	ATOM	1020		ASP			40.397	33.319	50.095	1.00-43.77	
35	ATOM	1021		ASP				34.123	49.334	1.00 46.50	
33	ATOM	1021	C	ASP			39.299	33.702	51.184	1.00 51.34	8
	ATOM	1023	0	ASP			39.302	30.176	47.898	1.00 38.62	6
	ATOM	1023	N				40.230	29.809	47.199	1.00 39.20	
	ATOM	1025	CA	SER SER			38.350	29.359	48.344	1.00 37.84	7
40	ATOM	1025					38.348	27.929	48.063	1.00 37.80	
70	ATOM	1027	CB	SER			37.240	27.240	48.878	1.00 34.28	6
		1027	OG C	SER			37.297	25.826	48.755	1.00 46.60	8
	ATOM ATOM		С	SER			38.164	27.639	46.581	1.00 38.41	6
		1029	0	SER			38.677	26.642	46.075	1.00 39.98	8
45	ATOM	1030	N			399	37.419	28.507	45.893	1.00 34.82	7
43	ATOM	1031	CA	PHE			37.181	28.325	44.462	1.00 35.96	6
	ATOM	1032	CB	PHE			35.873	28.983	44.015	1.00 35.75	6
	ATOM	1033	CG	PHE			34.632	28.216	44.403	1.00 39.30	6
	ATOM	1034	CD1				34.107	28.294	45.677	1.00 39.86	6
	ATOM	1035		PHE			34.018	27.393	43.488	1.00 36.81	6
50	ATOM	1036		PHE			32.961	27.557	46.013	1.00 41.25	6
	ATOM	1037	CE2				32.880	26.661	43.825	1.00 43.61	6
	ATOM	1038	CZ	PHE			32.354	26.740	45.087	1.00 40.34	6
	ATOM	1039	С	PHE			38.328	28.890	43.630	1.00 33.48	6
	ATOM	1040	0	PHE			38.867	28.200	42.756	1.00 26.86	8
55	MOTA	1041	N	LEU	Α	400	38.680	30.156	43.877	1.00 31.47	7
	MOTA	1042	CA	LEU	A	400	39.754	30.796	43.132	1.00 37.41	6
	ATOM	1043	CB	LEU	Α	400	40.179	32.100	43.814	1.00 34.24	6
	ATOM	1044	CG	LEU			39.239	33.265	43.628	1.00 35.10	6
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	·									
5			5 CD1	LEU	A 400	39.80	34.53	1 44.25		
	ATOM	104			A 400	39.06				
	ATOM	104	7 C		A 400	40.94	_			
	ATOM	104	8 0		A 400	41.36		:		
	ATOM	104	9 N		A 401					
10	ATOM				A 401	41.46			12.15	7
	ATOM				A 401	42.60				6
	ATOM					42.90			1.00 44.73	6
	ATOM	105			A 401	44.10			1.00 51.39	
	ATOM	105			A 401	45.37			1.00 50.11	
15					A 401	44.20		2 46.662		
13		1055	_		A 401	42.32	4 27.34			6
	ATOM	1056			A 401	43.05				
	ATOM	1057			A 402	41.26				8
	ATOM	1058		ALA	A 402	40.87				7
20	ATOM	1059		ALA .	A 402	39.522				6
20		1060) с	ALA .	A 402	40.798				6
	ATOM	1061	1 0		A 402	41.277		-		6
	ATOM	1062	2 N		A 403	40.200			1.00 32.14	8
	ATOM	1063	CA		A 403	40.052			1.00 31.07	7
	ATOM	1064	CB		A 403	39.379			1.00 29.90	6
25	ATOM	1065			A 403		-		1.00 27.03	6
	ATOM	1066		PHE A		38.943			1.00 26.97	6
	ATOM	1067		PHE A		38.228			1.00 25.55	6
	ATOM	1068				39.224			1.00 19.75	6
	ATOM	1069		PHE A	4 403	37.784			1.00 27.90	6
30	ATOM	1070	_	PHE A		38.780			1.00 22.56	6
	ATOM	1070		PHE A		38.063		35.640	1.00 22.24	6
	ATOM	1071		PHE P		41.429	27.756	38.719	1.00 28.82	6
	ATOM			PHE A		41.666	27.210	37.646	1.00 26.00	8
	ATOM	1073		GLU A		42.329	28.463		1.00 30.25	7
35		1074		GLU A		43.695	28.665	38.922	1.00 34.03	6
33	ATOM	1075		GLU À		44.513		39.983	1.00 34.03	
	ATOM	1076		GLU A		45.867		39.489	1.00 39.43	6
	ATOM	1077		GLU A		46.734	30.507	40.571	1.00 47.88	6
	ATOM	1078		GLU A		46.236	31.298	41.408		6
40	MOTA	1079	OE2 (GLU À	404	47.956	30.202	40.606	1.00 57.27	8
40	ATOM	1080	C (GLU A	404	44.352	27.322		1.00 63.85	8
	ATOM	1081		GLU A		44.936	27.112	38.634	1.00 36.01	6
	ATOM	1082	N F	HIS A	405	44.259	26.420	37.574	1.00 38.64	8
	ATOM	1083		IIS A		44.840	25.093	39.610	1.00 29.56	7
	ATOM	1084		IIS A		44.540		39.468	1.00 31.69	6
45	ATOM	1085		IIS A		45.292	24.228	40.694	1.00 33.75	6
	ATOM	1086	CD2 H	IIS A	405		24.657	41.908	1.00 34.75	6
	ATOM .	1087	ND1 H	TS A	405	46.198	25.640	42.130	1.00 34.58	6
	ATOM	1088	CE1 H	מ פדו	405	45.161	23.984	43.130	1.00 32.43	7
	ATOM	1089	NE2 H	א פבי	405	45.975	24.568	44.018	1.00 36.15	6
50	ATOM	1090				46.601	25.561	43.430	1.00 39.84	7
	ATOM	1091		IS A		44.274	24.445	38.225	1.00 34.21	6
	ATOM			IS A		45.029	23.949	37.386	1.00 37.06	8
	ATOM	1092		YR A		42.947	24.453	38.100	1.00 30.83	7
		1093		YR A		42.313	23.859		1.00 28.85	6
55	ATOM	1094		YR A		40.805	24.080		1.00 28.83	
دد	ATOM	1095	CG T	YR A	406	40.139	23.494		1.00 31.48	6
	ATOM	1096	CD1 T	YR A	406	40.073	22.123			6
	ATOM	1097	CE1 T	YR A	406	39.517	21.577		1.00 19.42	6
	ATOM	1098	CD2 T	YR A	406	39.646	24.313		1.00 23.80	6
							-1.313	54.704	1.00 21.81	6

-		1000	CE2 T	עם א	406	39.090	23.769	33.551	1.00 24.64	6
5	ATOM	1099		YR A		39.029		33.380	1.00 21.56	6
	ATOM	1100		YR A		38.489	21.850	32.236	1.00 24.96	8
	MOTA	1101				42.882	24.504	35.672	1.00 24.24	6
	MOTA	1102		YR A		42.958	23.872	34.621	1.00 27.08	8
_	MOTA	1103		YR A		43.253	25.784	35.807	1.00 25.76	7
10	MOTA	1104		LE A		43.824	26.548	34.705	1.00 33.75	6
	MOTA	1105		LE A		43.986	28.033	35.070	1.00 34.23	6
	MOTA	1106		LE A		44.967	28.712	34.139	1.00 32.46	6
	MOTA	1107		LE A		42.615	28.728	35.042	1.00 43.30	6
	ATOM	1108	CG1 I				28.602	33.694	1.00 40.40	6
15	MOTA	1109		LE A		41.896	25.973	34.256	1.00 39.03	6
	MOTA	1110		LE A		45.143	25.771	33.063	1.00 35.18	8
	MOTA	1111		LLE A		45.383	25.771	35.227	1.00 33.15	7
	MOTA	1112		ASN A		46.003	25.721	34.926	1.00 37.23	6
	MOTA	1113		ASN A		47.307		36.213	1.00 32.27	6
20	MOTA	1114		ASN A		48.107	25.017	36.936	1.00 33.56	6
	MOTA	1115		ASN A		48.346	26:362	36.320	1.00 33.30	8
	MOTA	1116		ASN A		48.827	27.335	38.231	1.00 31.33	7
	MOTA	1117		ASN A		48.038	26.403		1.00 31.23	6
	MOTA	1118		ASN A		47.205	23.892	34.136	1.00 33.14	8
25	ATOM	1119		ASN A		47.900	23.734	33.124	1.00 42.10	7
	ATOM	1120		TYR A		46.334	22.981	34.568	1.00 35.02	6
	MOTA	1121		TYR A		46.159	21.710	33.866	1.00 33.31	6
	ATOM	1122	CB	TYR F		45.051	20.859	34.507	1.00 34.41	6
	MOTA	1123	CG	TYR F		44.624	19.687	33.619	1.00 38.73	6
30	ATOM	1124		TYR F		45.563	18.765	33.155	1.00 47.16	6
	MOTA	1125		TYR A		45.186		32.321	1.00 47.18	6
	ATOM	1126		TYR A		43.292	19.515	33.232	1.00 40.20	6
	MOTA	1127	CE2			42.913		32.397	1.00 50.88	6
	MOTA	1128	CZ		A 409	43.863		31.946	1.00 53.14	8
35	MOTA	1129	OH		A 409	43.498		31.130	1.00 33.14	6
	MOTA	1130	С		A 409	45.760		32.424	1.00 30.10	8
	MOTA	1131	0		A 409	46.202		31.502	1.00 42.25	7
	ATOM	1132	N		A 410	44.872		32.272 30.984	1.00 42.23	
	ATOM	1133	CA		A 410	44.345	_			
40	MOTA	1134	CB		A 410	43.311		31.195		
	ATOM	1135	CG		A 410	41.994		31.795 30.675	1.00 34.32	
	MOTA	1136	CD		A 410	41.073	_			
	ATOM	1137	NE		A 410	40.888				
	MOTA	1138			A 410	40.177				
45	ATOM	1139			A 410	39.572				
	MOTA	1140) NH2		A 410	40.07				
	MOTA	1141	C		A 410	45.442				
	ATOM	1142	2 0		A 410	45.46				
	ATOM	1143	3 N	LYS	A 411	46.360				
50			4 CA	LYS	A 411	47.46	_			
	ATOM			LYS	A 411	48.64				
	MOTA			LYS	A 411	48.34				
	ATOM			LYS	A 411	49.60				
	ATOM				A 411	49.46				
55					A 411	50.74				
22	ATOM				A 411	47.03				
	ATOM	_			A 411	47.16				
	ATOM				A 412	46.45	8 26.943	28.82	3 1.00 54.6	7 7

5	MOTA	1153	CA	HIS	Α	412	45.984	27.722	27.705	1.00	48.67	6
	ATOM	1154	CB	HIS	Α	412	45.124	28.884	28.201	1.00	43.14	6
	ATOM	1155	CG	HIS	A	412	43.812	28.480	28.755		41.36	6
	ATOM	1156	CD2	HIS	Α	412	43.429	28.064	29.987		35.44	6
	ATOM	1157	ND1	HIS	Α	412	42.651	28.440	27.966		38.19	7
10	ATOM	1158	CE1	HIS	Α	412	41.648	28.014	28.723		34.75	6
	ATOM	1159	NE2			412	42.094	27.780	29.942		35.52	7
	ATOM	1160	С			412	47.231	28.303	27.101		46.35	6
	ATOM	1161	0			412	48.269	28.452	27.775		42.73	
	ATOM	1162	N			413	47.116	28.696	25.839			8
15	ATOM	1163	CA			413	48.234	29.290			48.92	7
••	ATOM	1164	CB			413	48.404		25.146		53.15	6
	ATOM	1165	CG			413	49.326	28.666	23.755		55.27	6
	ATOM	1166				413		29.446	22.886		58.77	6
	ATOM	1167				413	49.213	30.660	22.304		61.65	6
20	ATOM	1168				413	50.617	28.997	22.564		60.31	7
20	ATOM	1169				413	51.214	29.924	21.828		63.01	6
	ATOM	1170					50.386	30.941	21.658		62.93	7
		1170	C			413	47.932	30.768	24.998		53.19	6
	ATOM		0			413	47.639	31.301	23.934		54.93	8
25	ATOM	1172	N			414	47.964	31.413	26.139		53.77	7
23	ATOM	1173	CA			414	47.735	32.811	26.146		51.06	6
	ATOM	1174	CB			414	46.291	33.183	26.417		51.49	6
	ATOM	1175	CG1			414	46.186	34.715	26.603	1.00	45.22	6
	ATOM	1176				414	45.419	32.732	25.263		52.67	6
20	ATOM	1177	C			414	48.623	33.283	27.226	1.00	54.28	6
30	ATOM	1178	0			414	48.427	33.029	28.409		55.49	8
	ATOM	1179	N			415	49.706	33.863	26.733		56.28	7
	ATOM	1180	CA			415	50.721	34.484	27.557	1.00	57.83	6
	ATOM	1181	CB			415	51.268	35.675	26 .7 58	1.00	59.64	6
35	ATOM	1182	OG1			415	51.605	36.754	27.636		66.69	8
33	ATOM	1183	CG2			415	50.197	36.158	25.745		59.42	6
	ATOM	1184	C			415	50.146	35.049	28.879		56.98	6
	ATOM	1185	0		•	415	48.933	35.146	29.051		55.70	8
	ATOM	1186	N			416	51.068	35.330	29.795		57.44	7
40	ATOM	1187	CA			416	50.808	36.011	31.047	1.00	57.34	6
40	ATOM	1188	CB			416	51.346	37.422	30.708	1.00	61.35	6
	ATOM	1189	CG			416	51.872	38.237	31.821	1.00	69.78	6
	ATOM	1190				416	53.114		32.390	1.00	71.42	6
	ATOM	1191		HIS			51.135	39.263	32.416	1.00	72.49	7
4 =	ATOM	1192				416	51.914	39.884	33.290	1.00	75.50	6
45	ATOM	1193				416	53.099	39.323	33.291	1.00	73.91	7
	ATOM	1194	С			416	49.261	35.892	31.297	1.00	53.79	6
	ATOM	1195	0			416	48.499	36.779	30.902	1.00	52.81	8
	MOTA	1196	N	PHE	Α	417	48.806	34.779	31.911	1.00	48.05	7
	MOTA	1197	CA	PHE	Α	417	47.355	34.428	32.061	1.00	47.99	6
50	ATOM	1198	CB	PHE	Α	417	47.165	32.954	31.996		46.11	6
	MOTA	1199	CG	PHE	Α	417	45.835	32.590	31.399		44.27	6
	ATOM	1200	CD1	PHE	Α	417	45.680	32.720	30.046		41.79	6
	MOTA	1201	CD2	PHE	Α	417	44.758	32.135	32.164		40.23	6
	ATOM	1202		PHE			44.498	32.397	29.422		44.30	6
55	ATOM	1203		PHE			43.540	31.802	31.529		36.80	6
	ATOM	1204	CZ			417	43.427	31.928	30.144		40.69	6
	ATOM	1205	С	PHE			46.427	34.836	33.196		46.69	6
	ATOM	1206	0	PHE			46.147	36.004	33.331		43.35	8
								55.554		1.00		O

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5	ATCM	1207	N	TRP	Α	418	45.906	33.801	33.909	1.00 45.14	7
,	ATOM	1208	CA	TRP			44.982	33.867	35.065	1.00 44.89	6
	ATOM	1209	СВ	TRP			45.545	33.099	36.255	1.00 42.24	6
	ATOM	1210	CG	TRP			44.959	33.452	37.598	1.00 47.11	6
		1211	CD2				43.724	32.924	38.149	1.00 46.98	6
10	ATOM						43.534	33.565	39.413	1.00 48.94	6
10	ATOM	1212		TRP			42.777	31.986	37.688	1.00 45.23	6
	ATOM	1213		TRP				34.350	38.512	1.00 45.23	6
	MOTA	1214		TRP			45.434				7
	MOTA	1215		TRP			44.588	34.407	39.608	1.00 50.63	6
	MOTA	1216					42.441	33.270	40.238	1.00 45.46	
15	MOTA	1217		TRP			41.686	31.706	38.500	1.00 44.50	6
	ATOM	1218	CH2	TRP			41.511	32.335	39.753	1.00 47.55	6
	MOTA	1219	С	TRP			44.908	35.324	35.398	1.00 43.88	6
	ATOM	1220	0	TRP			43.797	35.839	35.702	1.00 43.17	8
	MOTA	1221	N			419	46.084	35.976	35.461	1.00 43.55	7
20	MOTA	1222	CD	PRO	Α	419	47.467	35.482	35.400	1.00 41.52	6
	ATOM	1223	CA	PRO	Α	419	46.009	37.396	35.758	1.00 41.48	6
	MOTA	1224	CB	PRO	A	419	47.436	37.884	35.535	1.00 39.21	6
	ATOM	1225	CG	PRO	Α	419	48.261	36.696	35.223	1.00 39.25	6
	ATOM	1226	С	PRO	A	419	44.960	38.090	34.817	1.00 36.28	6
25	ATOM	1227	0	PRO	A	419	44.208	38.978	35.237	1.00 37.08	8
	ATOM	1228	N	LYS	Α	420	44.915	37.701	33.540	1.00 35.96	7
	ATOM	1229	CA			420	43.977	38.287	32.575	1.00 40.82	6
	ATOM	1230	СВ			420	44.314	37.805	31.155	1.00 40.78	6
	ATOM	1231	CG			420	45.684	38.244	30.641	1.00 48.62	6
30	ATOM	1232	CD		•	420	45.904	37.781	29.206	1.00 55.12	6
50	ATOM	1233	CE			420	47.248	38.261	28.673	1.00 53.26	6
	ATOM	1234	NZ		•	420	47.448	37.884	27.222	1.00 52.69	7
	ATOM	1235	C			420	42.580	37.832	32.948	1.00 40.29	6
	ATOM	1236	0		•	420	41.656	38.626	32.982	1.00 39.66	8
35	ATOM	1237	N			421	42.461	36.537	33.245	1.00 38.33	7
33	ATOM	1238	CA			421	41.186	35.931	33.613	1.00 37.60	6
	ATOM	1239	CB			421	41.397	34.433	33.915	1.00 43.66	6
	ATOM	1240	CG			421	40.204	33.518	33.828	1.00 46.50	6
		1240		LEU			39.643	33.624	32.426	1.00 45.15	6
40	ATOM					421	40.595	32.094	34.131	1.00 51.31	6
40	ATOM	1242	CD2				40.575	36.664	34.808	1.00 31.51	6
	ATOM	1243	C		•	421				1.00 39.59	8
	MOTA	1244	0			421	39.371	36.910	34.837	1.00 40.00	7
	MOTA	1245	N			422	41.412	37.017	35.782	1.00 39.57	6
	MOTA	1246	CA			422	40.946	37.726	36.961		
45	MOTA	1247	СВ			422	42.085	37.890	37.971	1.00 41.79	6
	MOTA	1248	CG			422	42.424	36.671	38.798	1.00 42.74	6
	MOTA	1249				422	43.490	37.010	39.820	1.00 42.89	6
	MOTA	1250	CD2			422	41.168	36.216	39.523	1.00 39.27	6
	ATOM	1251	С			422	40.381	39.073	36.589	1.00 40.47	6
50	MOTA	1252	0	LEU	Α	422	39.428	39.525	37.210	1.00 47.83	8
	ATOM	1253	N	MET	Α	423	40.969	39.698	35.569	1.00 34.27	7
	ATOM	1254	CA	MET	Α	423	40.511	41.001	35.117	1.00 35.25	6
	ATOM	1255	СВ	MET	Α	423	41.427	41.553	34.028	1.00 32.56	6
	ATOM	1256	CG	MET	A	423	42.856	41.732	34.456	1.00 40.70	6
55	ATOM	1257	SD			423	43.707	43.101	33.619	1.00 47.65	16
	ATOM	1258	CE			423	43.348	42.776	31.848	1.00 47.16	6
	ATOM	1259	c			423		40.899	34.574	1.00 35.13	6
	ATOM	1260	Ö			423	38.315	41.829	34.696	1.00 29.85	8
	011	1200	-				33.313				_

5	ATOM	1261	N	LYS			38.791	39.752	33.975		31.56	7
	ATOM	1262	CA	LYS	Α	424	37.470	39.529	33.423	1.00	32.29	6
	MOTA	1263	CB	LYS	Α	424	37.446	38.205	32.658	1.00	30.56	6
	ATOM	1264	CG	LYS	Α	424	38.394	38.192	31.455	1.00	30.07	6
	ATOM	1265	CD	LYS			38.050	39.326	30.488	1.00	33.22	6
10	ATOM	1266	CE	LYS			39.032	39.433	29.322		28.75	6
	ATOM	1267	NZ	LYS			40.394	39.942	29.707		31.01	7
	ATOM	1268	C	LYS			36.418	39.558	34.524		29.26	6
	ATOM	1269	Ö	LYS			35.307	39.998	34.289		30.22	8
	ATOM	1270	N	VAL			36.796	39.098	35.719		23.53	7
15	ATOM	1271	CA	VAL			35.897	39.107	36.866		28.91	6
13	ATOM	1272	CB	VAL			36.541	38.460	38.094		29.44	6
	MOTA	1272	CG1	VAL			35.673	38.642	39.320		28.81	6
		1273	CG2	VAL			36.764	36.985	37.849			6
	ATOM										31.22	
20	ATOM	1275	С	VAL			35.512	40.548	37.161		32.03	6
20	ATOM	1276	0	VAL			34.350	40.839	37.429		31.95	8
	MOTA	1277	N	THR			36.496	41.444	37.124		33.61	7
	ATOM	1278	CA	THR			36.248	42.866	37.356		30.76	6
	MOTA	1279	CB			426	37.559	43.670	37.360		32.34	6
	ATOM	1280	OG1	THR		•	38.209	43.565	38.630		33.07	8
25	ATOM	1281	CG2			426	37.302	45.131	37.015		25.40	6
	MOTA	1282	С			426	35.363	43.324	36.211		32.53	6
	MOTA	1283	0			426	34.357	44.006	36.405		35.19	8
	ATOM	1284	N	ASP	•		35.763	42.929	35.006		28.83	7
	MOTA	1285	CA	ASP	•	-	35.011	43.272	33.810		35.12	6
30	MOTA	1286	CB			427	35.556	42.524	32.578		39.14	
	MOTA	1287	CG			427	36.837	43.103	32.057		45.80	6
	MOTA	1288		ASP	•		36.982	44.346	32.024		41.97	8
	MOTA	1289		ASP			37.735	42.333	31.616		50.06	8
	ATOM	1290	С			427	33.537	42.925	34.028	1.00	33.94	6
35	ATOM	1291	0	ASP	Α	427	32.659	43.712	33.702	1.00	38.02	8
	ATOM	1292	N	LEU	A	428	33.283	41.745	34.584	1.00	27.15	7
	MOTA	1293	CA	LEU	Α	428	31.925	41.293	34.850	1.00	29.99	6
	ATOM	1294	CB	LEU	A	428	31.924	39.786	35.133	1.00	22.49	6
	ATOM	1295	CG	LEU	Α	428	32.104	38.873	33.939	1.00	25.54	6
40	MOTA	1296	CD1	LEU	Α	428	32.202	37.421	34.353	1.00	20.60	6
	ATOM	1297	CD2	LEU	Α	428	30.920	39.083	33.029	1.00	17.24	6
	ATOM	1298	С	LEU	Α	428	31.276	42.057	35.991	1.00	28.94	6
	ATOM	1299	0			428	30.082	42.306	35.939		31.26	8
	ATOM	1300	N			429	32.059	42.423	37.011		27.64	7
45	ATOM	1301	CA			429	31.527	43.162	38.147	1.00	28.13	6
	ATOM	1302	СВ			429	32.564	43.298	39.264		29.59	6
	ATOM	1303	CG			429	32.818	42.040	40.080		34.85	6
	ATOM	1304	CD			429	33.588	42.360	41.367		47.18	6
	ATOM	1305	NE			429	34.093	41.175	42.049		57.93	7
50	MOTA	1306	CZ			429	33.327	40.210	42.547		63.62	6
50	MOTA	1307		ARG			31.998	40.270	42.396		60.71	7
	ATOM	1307		ARG			33.900	39.165	43.150		62.38	7
	MOTA	1309	С			429	31.099	44.536	37.707		29.81	6
55	ATOM	1310	0			429	30.044	45.009	38.101		30.81	8
55	ATOM	1311	N			430	31.941	45.176	36.901		29.64	7
	ATOM	1312	CA			430	31.644	46.502	36.383		34.72	6
	ATOM	1313	CB			430	32.745	46.955	35.434		34.97	6
	ATOM	1314	CG	MET	Α	430	33.937	47.597	36.080	1.00	45.34	6

5	ATOM	1315	SD	MET	A	430	33.520	49.120	36.937	1.00	52.55	16
	ATOM	1316	CE	MET	A	430	32.942	50.174	35.585		55.56	6
	ATOM	1317	С	MET	A	430	30.315	46.455	35.634		34.01	6
	ATOM	1318 -	0	MET	Α	430	29.455	47.295	35.854		37.29	8
	ATOM	1319	N	ILE	Α	431	30.180	45.468	34.740		29.99	7
10	ATOM	1320	CA	ILE	Α	431	28.954	45.269	33.969		28.82	6
	ATOM	1321	CB			431	28.962	43.936	33.211		27.39	6
	ATOM	1322	CG2			431	27.622	43.671	32.572		23.87	6
	ATOM	1323	CG1	ILE	Α	431	30.044	43.920	32.138		25.56	6
	ATOM	1324	CD1			431	29.989	42.703	31.244		17.29	6
15	ATOM	1325	С			431	27.769	45.269	34.907		29.49	6
	ATOM	1326	0			431	26.810	45.993	34.712		24.19	8
	ATOM	1327	N			432	27.839	44.435	35.936		25.25	7
	ATOM	1328	CA			432	26.748	44.343	36.890		30.38	6
	ATOM	1329	С			432	26.494	45.671	37.554		32.75	6
20	ATOM	1330	0			432	25.411	46.206	37.469		36.38	8
	ATOM	1331	N			433	27.514	46.189	38.221		26.77	7
	ATOM	1332	CA			433	27.428	47.459	38.910		26.48	6
	ATOM	1333	СВ			433	28.836	47.970	39.203		19.90	6
	ATOM	1334	C			433	26.663	48.502	38.114		30.73	6
25	ATOM	1335	0			433	25.773	49.164	38.635		31.60	8
	ATOM	1336	N			434	27.027	48.654	36.854		33.22	7
	ATOM	1337	CA			434	26.371	49.616	35.996		34.34	6
	ATOM	1338	СВ			434	27.047	49.612	34.711	1.00		6
	ATOM	1339	SG			434	27.789	50.811	34.285	1.00		16
30	ATOM	1340	C	CYS			24.974	49.198	35.612		34.09	6
	ATOM	1341	0	CYS			24.107	50.040	35.415	1.00		8
	ATOM	1342	N	HIS			24.756	47.898	35.447	1.00	34.30	7
	ATOM	1343	CA	HIS			23.453	47.423	35.042	1.00	35.44	6
	ATOM	1344	СВ	HIS			23.404	45.904	35.104	1.00	31.76	6
35	ATOM	1345	CG			435	22.099	45.351	34.675	1.00	32.03	6
	ATOM	1346	CD2	HIS			21.697	44.790	33.519		28.61	6
	MOTA	1347		HIS			20.941	45.482	35.452		28.48	7
	ATOM	1348	CE1				19.912	45.025	34.759		33.27	6
	ATOM	1349	NE2	HIS			20.345	44.597	33.583	1.00	31.57	7
40	ATOM	1350	С	HIS			22.400	47.974	35.972		32.74	6
	ATOM	1351	0	HIS			21.304	48.284	35.565		32.87	8
	ATOM	1352	N	ALA			22.777	48.046	37.241		31.01	7
	ATOM	1353	CA	ALA			21.910	48.563	38.266		29.91	6
	ATOM	1354	CB	ALA			22.661	48.595	39.580		21.23	6
45	ATOM	1355	С	ALA			21.475	49.969	37.884		33.86	6
	ATOM	1356	0	ALA			20.296	50.298	37.910		36.10	8
	ATOM	1357	N	SER			22.453	50.795	37.532		35.19	7
	ATOM	1358	CA	SER			22.172	52.167	37.140		33.03	6
	ATOM	1359	СВ	SER			23.441	52.815	36.603		35.31	6
50	ATOM	1360	OG	SER			23.203	54.151	36.193		44.99	8
	ATOM	1361	С	SER			21.110	52.158	36.055		38.39	6
	ATOM	1362	0	SER			20.049	52.745	36.204		37.54	8
	ATOM	1363	N	ARG			21.432	51.483	34.956		37.32	7
	ATOM	1364	CA	ARG			20.534	51.379	33.821		39.30	
55	ATOM	1365	СВ	ARG			21.114	50.402	32.786		42.97	6
	ATOM	1366	CG	ARG			22.343	50.402	32.766		42.97	6
	ATOM	1367	CD	ARG			21.955	52.134	31.251		41.72	6
	ATOM	1368	NE	ARG			20.964	51.839	30.237		45.23	6 7
	-							31.033	50.257	1.00	13.00	,

5	ATOM	1369	CZ	ARG	А	438	20.063	52.718	29.809	1.00 49.71	6
	ATOM	1370	NH1	ARG	Α	438	20.046	53.958	30.318	1.00 50.91	7
	ATOM	1371	NH2	ARG	Α	438	19.198	52.354	28.865	1.00 46.86	7
	ATOM	1372	С	ARG	Α	438	19.147	50.922	34.240	1.00 42.37	6
	ATOM	1373	0	ARG	Α	438	18.147	51.297	33.625	1.00 40.58	8
10	ATOM	1374	N			439	19.080	50.120	35.298	1.00 42.25	7
	MOTA	1375	CA			439	17.803	49.624	35.763	1.00 42.81	6
	ATOM	1376	СВ			439	17.975	48.794	37.013	1.00 42.18	6
	ATOM	1377	CG			439	16.739	48.053	37.413	1.00 42.48	6
	ATOM	1378		PHE			16.198	47.111	36.562	1.00 47.09	6
15	ATOM	1379		PHE			16.105	48.320	38.613	1.00 39.76	6
	MOTA	1380		PHE			15.047	46.427	36.905	1.00 49.17	6
	ATOM	1381		PHE			14.940	47.630	38.963	1.00 45.10	6
	ATOM	1382	CZ			439	14.411	46.683	38.098	1.00 46.36	6
	ATOM	1383	С			439	16.921	50.803	36.075	1.00 44.79	6
20	ATOM	1384	0			439	15.830	50.903	35.554	1.00 40.26	8
	ATOM	1385	N			440	17.410	51.681	36.951	1.00 42.77	7
	ATOM	1386	CA			440	16.660	52.871	37.344	1.00 42.96	6
	MOTA	1387	СВ			440	17.546	53.824	38.150	1.00 42.30	6
	ATOM	1388	CG			440	17.943	53.297	39.500	1.00 37.13	6
25	ATOM	1389		LEU			18.620	54.389	40.316	1.00 33.65	6
	ATOM	1390		LEU			16.679	52.837	40.216	1.00 35.42	6
	ATOM	1391	С			440	16.025	53.596	36.168	1.00 45.47	6
	ATOM	1392	Ō			440	14.809	53.750	36.126	1.00 52.48	8
	ATOM	1393	N			441	16.836	54.060	35.223	1.00 49.15	7
30	ATOM	1394	CA			441	16.277	54.725	34.063	1.00 54.76	6
	ATOM	1395	СВ			441	17.329	54.955	33.031	1.00 56.68	6
	ATOM	1396	CG			441	18.134	56.161	33.282	1.00 62.73	6
	ATOM	1397	CD2				18.468	57.216	32.499	1.00 65.73	6
	ATOM	1398	ND1	HIS			18.701	56.431	34.538	1.00 66.01	7
35	MOTA	1399	CE1	HIS	À	441	19.332	57.594	34.473	1.00 65.55	6
	MOTA	1400	NE2	HIS	Α	441	19.205	58.085	33.255	1.00 60.09	7
	MOTA	1401	С			441	15.244	53.822	33.481	1.00 55.93	6
	ATOM	1402	0	HIS	Α	441	14.149	54.263	33.170	1.00 57.33	8
	ATOM	1403	N	MET	A	442	15.605	52.549	33.313	1.00 57.81	7
40	MOTA	1404	CA	MET	Α	442	14.661	51.583	32.778	1.00 59.11	6
	ATOM	1405	CB	MET	Α	442	15.191	50.154	32.922	1.00 55.93	6
	ATOM	1406	CG	MET	Α	442	16.336	49.813	32.022	1.00 58.52	6
	ATOM	1407	SD	MET	Α	442	16.681	48.008	31.851	1.00 60.99	16
	MOTA	1408	CE	MET	Α	442	17.085	47.602	33.581	1.00 52.61	6
45	ATOM	1409	С	MET	Ą	442	13.339	51.727	33.534	1.00 60.31	6
	ATOM	1410	0	MET	À	442	12.266	51.560	32.968	1.00 58.18	8
	ATOM	1411	N	LYS	Α	443	13.425	52.054	34.818	1.00 61.45	7
	ATOM	1412	CA	LYS	A	443	12.236	52.202	35.626	1.00 64.90	6
	ATOM	1413	СВ	LYS			12.608	52.141	37.090	1.00 64.40	6
50	MOTA	1414	CG	LYS			11.461	51.748	37.959	1.00 69.12	6
	ATOM	1415	CD	LYS			12.068	51.551	39.257	1.00 71.14	6
	MOTA	1416	CE	LYS	A	443	11.368	51.897	40.091	1.00 73.43	6
	ATOM	1417	NZ	LYS			11.883	51.712	41.415	1.00 67.97	7
	ATOM	1418	С	LYS			11.513	53.514	35.348	1.00 67.29	6
55	ATOM	1419	0	LYS			10.390	53.700	35.780	1.00 67.90	8
	ATOM	1420	N	VAL			12.171	54.429	34.629	1.00 66.57	7
	ATOM	1421	CA	VAL			11.575	55.719	34.297	1.00 64.76	6
	ATOM	1422	СВ	VAL			12.569	56.869	34.560	1.00 62.76	6
					-		-				-

5	ATOM	1423	CG1	VAL	A	444	11.952	58.195	34.174	1.00	64.00	6
	ATOM	1424	CG2	VAL	A	444	12.999	56.891	36.035	1.00	59.27	6
	ATOM	1425	С	VAL	А	444	11.043	55.730	32.861	1.00	68.61	6
	ATOM	1426	0	VAL	A	444	9.937	56.210	32.612	1.00	70.60	8
	MOTA	1427	N	GLU	А	445	11.814	55.173	31.935	1.00	70.71	7
10	ATOM	1428	CA	GLU	A	445	11.457	55.152	30.514	1.00	71.45	6
	ATOM	1429	CB	GLU	Α	445	12.725	55.255	29.664		72.36	6
	ATOM	1430	CG	GLU	Α	445	13.598	56.429	30.022		40.00	6
	MOTA	1431	CD	GLU	Α	445	14.875	56.472	29.239		40.00	6
	ATOM	1432	OE1	GLU	Α	445	15.155	55.565	28.414		40.00	8
15	ATOM	1433	OE2	GLU	A	445	15.663	57.430	29.430		40.00	8
	ATOM	1434	С	GLU	Α	445	10.724	53.912	30.049		71.46	6
	ATOM	1435	0	GLU	Α	445	10.536	53.701	28.844		73.02	8
	ATOM	1436	N	CYS			10.301	53.099	30.999		71.12	7
	ATOM	1437	CA	CYS			9.628	51.899	30.634		70.83	6
20	ATOM	1438	CB	CYS			10.595	50.719	30.687		71.05	6
	ATOM	1439	SG	CYS			12.009	50.842	29.573		72.83	16
	ATOM	1440	С	CYS			8.454	51.671	31.535		71.91	6
	ATOM	1441	0	CYS			8.495	52.014	32.728		72.06	8
	ATOM	1442	N	PRO			7.372	51.133	30.978		73.12	7
25	ATOM	1443	CD	PRO			7.267	50.764	29.560		72.88	6
	ATOM	1444	CA	PRO			6.150	50.853	31.740		74.22	6
	MOTA	1445	СВ	PRO			5.187	50.281	30.714		72.98	6
	ATOM	1446	CG	PRO			5.875	50.271	29.437		74.77	6
	ATOM	1447	C	PRO			6.435	49.843	32.831		75.94	6
30	ATOM	1448	0	PRO			7.181	48.908	32.612		76.67	8
	ATOM	1449	N	THR		•	5.820	50.002	33.997		76.91	7
	ATOM	1450	CA	THR			6.024	49.066	35.113		78.24	6
	ATOM	1451	СВ	THR			5.528	49.734	36.401		81.33	6
	ATOM	1452	OG1				4.105	49.917	36.328		84.46	8
35	ATOM	1453	CG2	THR			6.192	51.081	36.585		83.51	6
	ATOM	1454	С	THR			5.113	47.912	34.755		77.42	6
	MOTA	1455	0	THR			4.915	46.995	35.519		77.65	8
	ATOM	1456	N	GLU			4.539	48.021	33.565		76.29	7
	ATOM	1457	CA	GLU			3.630	47.023	33.024		75.03	6
40	MOTA	1458	СВ	GLU			2.600	47.773	32.191		74.62	6
	MOTA	1459	CG	GLU			2.145	47.051	31.001		40.00	6
	ATOM	1460	CD	GLU			1.297	47.889	30.178		40.00	6
	ATOM	1461		GLU			1.479	49.137	30.146		40.00	8
	ATOM	1462		GLU			0.424	47.322	29.497		40.00	8
45	ATOM	1463	С	GLU			4.434	46.036	32.179		73.49	6
	ATOM	1464	0	GLU		•	3.882	45.142	31.559		70.24	8
	ATOM	1465	N	LEU			5.747	46.224	32.161		70.80	7
	ATOM	1466	CA	LEU			6.608	45.347	31.378		68.82	
	ATOM	1467	СВ	LEU		•	7.301	46.154	30.277		71.91	6
50	ATOM	1468	CG	LEU			6.464	46.134				6
20	ATOM	1469		LEU			7.337		29.217		76.62	6
	ATOM	1470		LEU				47.662 45.750	28.328		77.95	6
	ATOM	1471					5.786		28.415		76.46	6
	ATOM	1471	C	LEU LEU			7.669	44.673	32.243		66.22	6
55	ATOM	1472	О И				8.427	43.841	31.752		66.01	8
J.J	ATOM	1473		PHE			7.705	45.039	33.530		61.96	7
	ATOM		CA	PHE			8.681	44.506	34.480		58.44	6
		1475	CB	PHE			9.041	45.562	35.540		61.34	6
	ATOM	1476	CG	PHE	A	451	9.873	46.717	35.008	1.00	63.02	6

_												
5				l PHE			9.426	47.50	7 33.963	3 1 00	62.92	_
	ATOM	1478	CD2	2 PHE	Ά	451	11.089					6
	ATOM	1479	CE	l PHE	Α	451	10.199				63.07	6
	ATOM	1480		PHE			11.860			-	65.12	6
	ATOM					451					64.66	6
10				PHE			11.410				67.12	6
	ATOM						8.259			1.00	56.41	6
				PHE			7.641		36.331		56.56	8
	ATOM			PRO			8.555	42.045	34.755		53.28	7
	ATOM	1485		PRO			9.177	41.689			50.46	6
	ATOM	1486		PRO	Α	452	8.153				50.26	
15	ATOM	1487	CB	PRO	Α	452	8.739					6
	ATOM	1488	CG	PRO	Α	452	9.178				49.19	6
	ATOM	1489	С	PRO			8.770				45.89	6
	ATOM	1490		PRO							49.62	6
	ATOM	1491		PRO			9.867				52.35	8
20	ATOM	1492					8.139			1.00	51.50	7
	ATOM			PRO			7.001		37.797	1.00	49.66	6
		1493		PRO			8.610	40.528	39.323		50.89	6
	ATOM	1494		PRO			7.675	39.659			51.49	6
	ATOM	1495		PRO	Ą	453	6.703	39.141		_	50.82	
	ATOM	1496	С	PRO	A	453	10.015	40.084				6
25	ATOM	1497	0	PRO	Α	453	10.876	40.900			50.99	6
	ATOM	1498	N	LEU .			10.255	38.781			54.17	8
	ATOM	1499	CA	LEU .			11.585		39.423		51.21	7
	ATOM	1500	CB	LEU			11.813	38.298	39.674		47.17	6
	ATOM	1501	CG	LEU				36.962	38.975		44.44	6
30	ATOM	1502	CD1				13.167	36.375	39.289		41.33	6
	ATOM	1503		LEU Z			13.524	36.638	40.720		35.93	6
	ATOM	1504	C				13.169	34.907	38.992		34.79	6
	ATOM	1505		LEU Z			12.541	39.375	39.182	1.00	42.25	6
	ATOM	1506	0	LEU A			13.477	39.718	39.886	1.00	40.82	8
35	ATOM		N	PHE 2			12.270	39.957	38.011	1.00		7
55		1507	CA	PHE A			13.133	41.005	37.473	1.00		6
	ATOM	1508	CB	PHE A			12.527	41.592	36.192	1.00		6
	ATOM	1509	CG	PHE A			13.433	42.565	35.467	1.00		6
	ATOM	1510		PHE A			14.715	42.189	35.135	1.00		6
	ATOM	1511	CD2	PHE A	4	155	12.999	43.840	35.126	1.00		
40	ATOM	1512	CE1	PHE P	4	155	15.557	43.059	34.466			6
•	ATOM	1513	CE2	PHE A	4	155	13.848	44.716		1.00		6
	MOTA	1514					15.129		34.452	1.00		6
	ATOM	1515		PHE A			13.123	44.322	34.126	1.00		6
	ATOM	1516		PHE A				42.085	38.534	1.00		6
45	ATOM	1517		LEU A			14.361	42.323	39.034	1.00 3		8
	ATOM	1518					12.155	42.735	38.849	1.00 4	13.92	7
	ATOM	1519		LEU A			12.122	43.803	39.840	1.00 4	14.08	6
	ATOM			LEU A			10.680	44.251	40.093	1.00 5		6
		1520		LEU A			10.062	45.242	39.144	1.00 5		6
60	ATOM	1521		LEU A			8.598	45.432	39.450	1.00 5		6
50	ATOM	1522		LEU A			10.807	46.548	39.295	1.00 5		
	ATOM	1523	C ;	LEU A	4	56	12.739	43.355	41.136	1.00 4		6
	ATOM	1524		LEU A			13.597	44.022	41.685			6
	ATOM	1525		GLU A			11.973	41.761		1.00 4		8
	ATOM	1526		GLU A			12.475		41.851	1.00 4		7
55	ATOM	1527		GLU A				41.179	43.105	1.00 4		6
	ATOM	1528		GLU A			14.005	41.236	43.132	1.00 4		6
	ATOM	1529		SLU A			14.583	41.724	44.117	1.00 4		8
	ATOM	1530		GLU A			12.024	39.723	43.223	1.00 5		6
			(TO A	4.	<i>)</i>	11.114	39.476	44.427	1.00 2	0.00	6

						10 007	27 004	44.648	1.00 20.00	6
5	MOTA	1531		LU A		10.807		44.311	1.00 20.00	8
	ATOM	1532		LU A		11.673	•		1.00 20.00	8
	MOTA	1533		LU A		9.683	=	45.172	1.00 20.00	7
	MOTA	1534		AL A		14.928		41.903	1.00 43.21	6
	MOTA	1535		AL A		16.412	41.094	41.868	1.00 44.93	6
10	ATOM	1536		AL A		16.881	40.306	40.642	1.00 44.83	6
	ATOM	1537		JAL A		18.365	40.106	40.698	1.00 49.72	6
	MOTA	1538		JAL A		16.185	38.979	40.558	1.00 40.89	6
	MOTA	1539		JAL A		17.130	42.420	41.877	1.00 42.72	8
	ATOM	1540		VAL A		18.061	42.617	42.658	1.00 42.88	7
15	MOTA	1541		PHE A		16.713	43.325	41.010	1.00 44.55	6
	ATOM	1542		PHE A		17.385	44.606	40.892		6
	MOTA	1543		PHE A		17.281	45.104	39.494	1.00 43.60 1.00 40.79	6
	MOTA	1544		PHE A		17.915	44.190	38.547		6
	MOTA	1545		PHE A		17.325	42.983	38.244	1.00 41.01	6
20	ATOM	1546		PHE A		19.153	44.483	38.054	1.00 39.48	6
	ATOM	1547	CE1	PHE A	459	17.988	42.081	37.441	1.00 40.62	6
	MOTA	1548		PHE A		19.814	43.589	37.257	1.00 36.87	6
	MOTA	1549		PHE A		19.233	42.385	36.940	1.00 36.39	6
	ATOM	1550		PHE A		16.837	45.648	41.744	1.00 52.71	8
25	ATOM	1551		PHE A		17.492	46.682	42.017	1.00 51.34	7
	ATOM	1552		GLU P		15.606	45.422	42.161	1.00 62.92	6
	ATOM	1553	CA	GLU F		15.066	46.428	42.965	1.00 69.33 1.00 72.95	6
	MOTA	1554	CB	GLU F		13.552	46.352	43.094	1.00 72.95	6
	MOTA	1555	CG	GLU A		12.978	47.767	42.957	1.00 78.33	6
30	MOTA	1556	CD	GLU A		12.246	48.261	44.157	1.00 82.97	8
	MOTA	1557		GLU A		12.471	47.759	45.281	1.00 88.28	8
	ATOM	1558	OE2	GLU A		11.422	49.200	44.017 44.272	1.00 34.80	6
	ATOM	1559	С	GLU Z		15.736		44.272	1.00 74.51	8
	MOTA	1560	0	GLU A		16.187			1.00 74.51	7
35	MOTA	1561	N		A 461		47.373 47.505	46.173	1.00 84.19	
	ATOM	1562	CA		A 461	16.415		46.471	1.00 85.82	6
	MOTA	1563			A 461	16.394		45.276	1.00 89.62	6
	MOTA	1564			A 461	16.801		44.086		8
	MOTA	1565		ASP		16.692 17.239		45.482		8
40	MOTA	1566		ASP		15.639		47.214	1.00 86.80	6
•	MOTA	1567			A 461	16.245				8
	MOTA	1568			A 461	14.457	_			8
	ATOM	1569	OXT	ASP	A 461	14.45/	47.020	17,101		
	TER	_			D 011	-20.802	66.251	39.780	1.00 46.72	6
45	MOTA	1			B 211	-19.566				
	ATOM	2			B 211	-18.264				
	MOTA	3			B 211	-18.043				
	MOTA	4			B 211	-19.008				
	MOTA				B 211	-22.418				
50			5 C		B 211	-23.35				
	ATOM		7 0		B 211	-20.74				
	MOTA		8 N		B 211					
	MOTA		9 CA		B 211	-20.99				
	ATOM				B 212	-22.61 -21.52				
55					B 212	-21.52 -23.94				
	MOTA				B 212					
	ATOM				B 212	-23.65 -22.2 <u>2</u>				
	ATOM	1	4 CG	PRO	В 212	-44.44	U /1.7/7			

ATOM 17 N GLU B 213	_										
ATOM 16 O PRO B 212 -24.350 70.045 38.696 1.00 34.64 8 ATOM 17 N GLU B 213 -26.058 69.424 40.032 1.00 40.31 7 ATOM 18 CA GLU B 213 -27.081 69.290 39.003 1.00 40.387 6 ATOM 20 CG GLU B 213 -27.081 69.290 39.265 1.00 45.166 67 ATOM 21 CD GLU B 213 -27.082 66.709 39.286 1.00 47.60 68 ATOM 22 CG GLU B 213 -27.082 66.709 39.286 1.00 47.60 68 ATOM 23 OE2 GLU B 213 -27.887 65.244 39.199 1.00 50.68 68 ATOM 24 C GLU B 213 -27.882 64.516 38.442 1.00 49.06 88 ATOM 25 O GLU B 213 -27.924 70.576 39.886 1.00 45.96 89.204 40.000 49.06 88 ATOM 25 O GLU B 213 -27.924 70.576 39.886 1.00 45.96 89.204 40.000 49.89 89.206 1.00 45.96 89.206 40.000 49.89 89.206 1.00 45.96 89.206 40.000 49.89 89.206 1.00 45.96 89.206 40.000 49.200	5		1	5 C	PRO	B 212	-24.79	8 69 77	2 30 00-	7 1 00 20 7	
ATOM 18 CA GLU B 213			1	6 0							
ATOM 18 CA GLU B 213		MOTA	1	7 N							-
ATOM 19 CB GLU B 213		ATOM	18	B CA							
ATOM		ATOM	19		_						
ATOM 21 CD CIU B 213	10	ATOM									
ATOM 23 OE2 GIU B 213 -28.847 65.244 39.886 1.00 59.18 8 ATOM 24 OE2 GIU B 213 -27.924 64.516 38.442 1.00 49.06 8 6 ATOM 25 O GIU B 213 -27.924 70.576 39.080 1.00 45.96 8 6 ATOM 25 O GIU B 213 -27.924 70.576 39.080 1.00 45.96 8 6 ATOM 27 CD PRO B 214 -29.484 69.635 37.446 1.00 49.06 8 ATOM 28 CA PRO B 214 -29.484 69.635 37.446 1.00 49.06 8 ATOM 29 CB PRO B 214 -29.484 69.635 37.446 1.00 49.89 6 ATOM 30 CG PRO B 214 -30.597 71.639 37.210 1.00 45.40 6 ATOM 31 C PRO B 214 -30.597 71.639 37.210 1.00 45.40 6 ATOM 31 C PRO B 214 -30.597 71.639 39.535 1.00 45.40 6 ATOM 33 N THR B 215 -31.180 73.515 39.506 1.00 49.89 6 ATOM 33 N THR B 215 -31.180 73.515 39.506 1.00 49.89 6 ATOM 36 OGI THR B 215 -31.443 75.420 41.091 1.00 44.49 8 ATOM 37 CG2 THR B 215 -31.443 75.420 41.091 1.00 44.66 6 ATOM 38 C THR B 215 -32.249 76.464 40.652 1.00 49.36 6 ATOM 39 O THR B 215 -33.366 74.239 40.114 1.00 52.26 8 ATOM 35 C THR B 215 -33.366 74.239 40.114 1.00 52.26 8 ATOM 36 C THR B 215 -33.366 74.239 40.114 1.00 52.26 8 ATOM 40 C ASP B 216 -33.562 74.868 39.078 1.00 53.48 8 ATOM 40 C ASP B 216 -36.674 74.005 41.650 1.00 78.57 6 ATOM 43 C ASP B 216 -36.674 74.005 41.650 1.00 78.07 6 ATOM 44 ODI ASP B 216 -36.674 74.005 41.650 1.00 78.07 6 ATOM 46 C ASP B 216 -37.675 72.991 41.710 1.00 78.07 6 ATOM 47 O ASP B 216 -37.675 72.991 41.710 1.00 78.07 6 ATOM 48 N GLU B 217 -34.954 75.999 39.353 1.00 53.48 8 ATOM 50 CB GLU B 217 -34.954 75.999 39.353 1.00 53.37 6 ATOM 50 CB GLU B 217 -34.954 75.999 39.353 1.00 53.37 6 ATOM 50 CB GLU B 217 -34.954 77.999 39.353 1.00 54.92 77 ATOM 50 CB GLU B 217 -34.954 77.999 39.353 1.00 54.92 77 ATOM 50 CB GLU B 217 -34.954 77.999 39.353 1.00 40.00 8 ATOM 60 CG GLU B 218 -34.365 77.619 39.699 1.00 40.00 6 ATOM 60 CG GLU B 218 -34.365 77.6991 37.945 1.00 40.00 8 ATOM 60 CG GLU B 218 -34.365 77.6991 37.945 1.00 40.00 8 ATOM 60 CG GLU B 218 -32.293 77.6991 37.945 1.00 40.00 8 ATOM 60 CG GLU B 218 -32.395 75.686 34.405 1.00 44.71 6 ATOM 60 CG GLU B 218 -32.395 75.686 34.405 1.00 44.71 6 ATOM 60 CG GLU B 218 -32.395 7											
ATOM 24 CE GLU B 213					_	D 213					
ATOM 24 C GLU B 213					T GTO	D 213					
15											
ATOM 26 N PRO B 214	15								39.080		_
ATOM 27 CD PRO B 214	13						-27.624	71.467	39.859		_
ATOM 28 CA PRO B 214 -29.484 69.635 37.446 1.00 46.44 6 ATOM 29 CB PRO B 214 -30.799 71.639 37.210 1.00 47.52 6 ATOM 30 CG PRO B 214 -30.597 71.595 36.805 1.00 49.89 6 ATOM 31 C PRO B 214 -30.597 71.595 40.483 1.00 44.49 8 ATOM 33 N THR B 215 -31.180 73.515 39.506 1.00 49.20 6 ATOM 35 CB THR B 215 -31.180 73.515 39.506 1.00 49.36 6 ATOM 36 CG THR B 215 -31.443 75.420 41.091 1.00 44.86 6 ATOM 37 CG2 THR B 215 -32.249 76.464 40.534 1.00 52.26 8 ATOM 38 C THR B 215 -33.386 74.239 40.114 1.00 52.51 6 ATOM 39 O THR B 215 -33.386 74.239 40.114 1.00 52.51 6 ATOM 40 N ASP B 216 -34.387 73.741 40.829 1.00 58.81 7 ATOM 41 CA ASP B 216 -36.674 74.005 40.485 1.00 61.51 6 ATOM 42 CB ASP B 216 -36.674 74.005 40.485 1.00 61.51 6 ATOM 43 CG ASP B 216 -36.674 74.005 40.652 1.00 78.07 6 ATOM 44 ODI ASP B 216 -36.674 75.472 39.40 114 1.00 52.51 6 ATOM 45 OD2 ASP B 216 -36.674 74.005 40.652 1.00 82.31 8 ATOM 46 C ASP B 216 -36.674 75.2981 41.710 1.00 78.07 6 ATOM 48 N GLU B 217 -34.851 77.599 39.984 1.00 58.42 6 ATOM 47 O ASP B 216 -36.828 72.588 40.652 1.00 82.31 8 ATOM 48 N GLU B 217 -34.851 77.599 39.985 1.00 40.00 6 ATOM 50 CB GLU B 217 -34.851 77.599 39.9353 1.00 58.45 97 ATOM 51 CG GLU B 217 -34.851 77.599 39.9353 1.00 53.37 8 ATOM 54 OC2 GLU B 217 -34.851 77.599 39.353 1.00 53.55 8 ATOM 55 CB GLU B 217 -34.851 77.599 39.353 1.00 53.55 8 ATOM 54 OC2 GLU B 217 -34.851 77.599 39.353 1.00 53.55 6 ATOM 55 CB GLU B 217 -34.851 77.599 39.353 1.00 40.00 6 ATOM 50 CB GLU B 218 -33.366 75.793 36.981 1.00 40.00 8 ATOM 50 CB GLU B 218 -33.366 75.793 36.981 1.00 40.00 6 ATOM 50 CG GLU B 218 -33.366 75.793 36.981 1.00 40.00 6 ATOM 50 CG GLU B 218 -33.366 75.793 36.981 1.00 40.00 8 ATOM 60 CG GLU B 218 -32.318 76.359 37.945 1.00 40.00 6 ATOM 61 CD GLU B 218 -32.318 76.359 37.945 1.00 40.00 6 ATOM 62 CGLU B 218 -33.366 75.793 36.981 1.00 40.00 6 ATOM 64 C GLU B 218 -33.065 75.793 36.981 1.00 40.00 6 ATOM 65 O GLU B 218 -33.066 75.793 36.981 1.00 44.02 7 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 66 N TRP B 219 -33.669 75.6											
ATOM 28 CA PRO B 214							-29.484	69.635			
ATOM 29 CB PRO B 214 -30.799 71.639 37.210 1.00 45.40 6 ATOM 31 C PRO B 214 -30.530 70.257 36.805 1.00 49.89 6 ATOM 32 O PRO B 214 -30.574 72:330 39.535 1.00 45.70 6 ATOM 32 O PRO B 214 -30.597 71.595 40.483 1.00 44.49 8 ATOM 34 CA THR B 215 -31.180 73.515 39.506 1.00 49.36 6 ATOM 35 CB THR B 215 -31.965 74.036 40.652 1.00 49.36 6 ATOM 36 OG1 THR B 215 -31.443 75.420 41.091 1.00 44.86 6 ATOM 37 CG2 THR B 215 -31.443 75.420 41.091 1.00 54.86 6 ATOM 38 C THR B 215 -33.386 74.239 40.114 1.00 52.26 8 ATOM 39 O THR B 215 -33.386 74.239 40.114 1.00 52.51 6 ATOM 39 O THR B 215 -33.386 74.239 40.114 1.00 53.48 8 ATOM 40 N ASP B 216 -35.562 74.868 39.078 1.00 53.48 8 ATOM 41 CA ASP B 216 -35.795 73.865 40.435 1.00 61.51 6 ATOM 42 CB ASP B 216 -35.795 73.865 40.435 1.00 61.51 6 ATOM 44 OD1 ASP B 216 -36.674 74.005 41.650 1.00 70.57 6 ATOM 45 OD2 ASP B 216 -37.675 72.981 41.710 1.00 78.07 6 ATOM 46 C ASP B 216 -37.675 72.981 41.710 1.00 78.07 6 ATOM 47 O ASP B 216 -37.883 72.567 42.830 1.00 86.55 8 ATOM 46 C ASP B 216 -36.847 75.317 38.827 1.00 54.92 7 ATOM 48 N GLU B 217 -34.954 75.979 39.984 1.00 554.92 7 ATOM 50 CB GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 50 CB GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 50 CB GLU B 217 -34.164 78.264 40.251 1.00 50.33.37 6 ATOM 50 CB GLU B 217 -34.164 78.264 40.251 1.00 40.00 6 ATOM 50 CB GLU B 217 -34.165 77.612 37.018 1.00 54.33 8 ATOM 50 CB GLU B 217 -34.165 77.612 37.018 1.00 54.33 8 ATOM 50 CB GLU B 217 -34.252 77.63 37.957 1.00 54.33 8 ATOM 50 CB GLU B 218 -33.063 76.572 37.839 1.00 45.43 6 ATOM 50 CB GLU B 218 -33.063 76.572 37.839 1.00 40.00 6 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 40.00 6 ATOM 60 CG GLU B 218 -32.866 74.967 38.449 1.00 37.61 8 ATOM 66 CG GLU B 218 -33.067 76.901 37.945 1.00 40.00 40.00 6 ATOM 66 CG GLU B 218 -32.866 74.967 37.439 36.131 1.00 44.02 7 ATOM 66 CG GLU B 218 -32.935 75.666 34.405 1.00 44.71 6 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6							-29.843			•	_
ATOM 30 CG PRO B 214	•										
ATOM 31 C PRO B 214 -30.574 72:330 39.535 1.00 49.570 6 ATOM 32 O PRO B 214 -30.597 71.595 40.483 1.00 44.49 8 ATOM 33 N THR B 215 -31.180 73.515 39.506 1.00 45.24 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	20		30	CG	PRO	B 214					-
ATOM 32 O PRO B 214 ATOM 33 N THR B 215 ATOM 34 CA ATOM 34 CA THR B 215 ATOM 35 CB THR B 215 ATOM 35 CB THR B 215 ATOM 36 CGI THR B 215 ATOM 37 CG2 THR B 215 ATOM 38 C ATOM 37 CG2 THR B 215 ATOM 38 C ATOM 39 O THR B 215 ATOM 40 N ASP B 216 ATOM 41 CA ASP B 216 ATOM 43 CG ASP B 216 ATOM 43 CG ASP B 216 ATOM 44 ODI ASP B 216 ATOM 45 OD2 ASP B 216 ATOM 46 C ASP B 216 ATOM 47 O ASP B 216 ATOM 48 N ACUB 217 ATOM 49 CA ATOM 50 CB ATOM 51 CG ATOM 51 CG ATOM 51 CG ATOM 52 CD ATOM 51 CG ATOM 52 CD ATOM 53 CEB UB 217 ATOM 54 CB ATOM 55 CG ATOM 55 CB ATOM 56 CB ATOM 57 N ATOM 57 N ATOM 58 CA ATOM 59 CB ATOM 66 N ATOM 66 CB ATOM 67 CA ATOM 67 CA ATOM 67 CA ATOM 67 CA ATOM 68 CB ATOM 66 N ATOM 67 CA ATOM 66 N ATOM 67 CA ATO		ATOM	31	С							
ATOM 33 N THR B 215		ATOM	32	0				-			_
ATOM 34 CA THR B 215		ATOM	33	N					-		_
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ATOM 36 OG1 THR B 215 -32.249 76.464 40.534 1.00 52.26 6 ATOM 37 CG2 THR B 215 -30.011 75.617 40.659 1.00 39.43 6 ATOM 38 C THR B 215 -33.386 74.239 40.114 1.00 52.51 6 ATOM 40 N ASP B 216 -34.387 73.741 40.829 1.00 53.48 8 ATOM 41 CA ASP B 216 -34.387 73.741 40.829 1.00 53.48 8 ATOM 42 CB ASP B 216 -35.795 73.865 40.435 1.00 61.51 6 ATOM 43 CG ASP B 216 -36.674 74.005 41.650 1.00 70.57 6 ATOM 44 OD1 ASP B 216 -37.675 72.981 41.710 1.00 78.07 6 ATOM 45 OD2 ASP B 216 -37.983 72.567 42.830 1.00 82.31 8 ATOM 46 C ASP B 216 -37.983 72.567 42.830 1.00 86.55 8 ATOM 47 O ASP B 216 -36.847 75.317 38.827 1.00 56.85 8 ATOM 49 CA GLU B 217 -34.954 75.979 39.984 1.00 54.92 7 ATOM 50 CB GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 50 CB GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 51 CG GLU B 217 -34.104 78.264 40.251 1.00 40.00 6 ATOM 55 CG GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 56 O GLU B 217 -34.232 77.163 37.957 1.00 53.55 6 ATOM 56 O GLU B 218 -33.063 76.572 37.839 1.00 40.00 8 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.00 8 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.01 8 ATOM 60 CG GLU B 218 -33.066 76.728 37.801 1.00 40.01 8 ATOM 60 CG GLU B 218 -33.014 75.475 35.610 1.00 44.01 6 ATOM 60 CG GLU B 218 -33.014 75.475 35.610 1.00 44.01 6 ATOM 60 CG ATPP B 219 -34.368 73.490 35.290 1.00 46.97 6	25	ATOM	35								6
ATOM 37 CG2 THR B 215		ATOM									6
ATOM 38 C THR B 215 -33.386 74.239 40.114 1.00 52.51 6 ATOM 39 O THR B 215 -33.562 74.868 39.078 1.00 53.48 8 ATOM 40 N ASP B 216 -34.387 73.741 40.829 1.00 58.81 7 ATOM 41 CA ASP B 216 -35.795 73.865 40.435 1.00 61.51 6 ATOM 43 CG ASP B 216 -36.674 74.005 41.650 1.00 70.57 6 ATOM 44 ODI ASP B 216 -36.674 74.005 41.650 1.00 70.57 6 ATOM 45 OD2 ASP B 216 -37.675 72.981 41.710 1.00 78.07 6 ATOM 46 C ASP B 216 -37.983 72.567 42.830 1.00 86.55 8 ATOM 47 O ASP B 216 -35.920 75.123 39.648 1.00 58.42 6 ATOM 49 CA GLU B 217 -34.954 75.979 39.984 1.00 56.85 8 ATOM 49 CA GLU B 217 -34.851 77.259 39.353 1.00 55.37 6 ATOM 50 CB GLU B 217 -34.104 78.264 40.251 1.00 51.02 6 ATOM 50 CB GLU B 217 -34.104 78.264 40.251 1.00 40.00 6 ATOM 50 CB GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 50 CE GLU B 217 -34.232 77.163 37.957 1.00 40.00 6 ATOM 50 CE GLU B 217 -34.232 77.163 37.957 1.00 40.00 8 ATOM 50 CE GLU B 217 -34.232 77.163 37.957 1.00 40.00 8 ATOM 50 CE GLU B 218 -33.363 76.572 37.839 1.00 49.20 7 ATOM 50 CE GLU B 218 -33.363 76.572 37.839 1.00 49.20 7 ATOM 50 CE GLU B 218 -33.3063 76.572 37.839 1.00 49.20 7 ATOM 50 CE GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 50 CE GLU B 218 -33.063 76.572 37.839 1.00 40.86 6 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.86 6 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.86 6 ATOM 60 CG GLU B 218 -33.065 76.728 37.801 1.00 40.86 6 ATOM 61 CD GLU B 218 -33.065 76.728 37.801 1.00 40.86 6 ATOM 62 OEI GLU B 218 -33.065 76.728 37.801 1.00 40.86 6 ATOM 64 C GLU B 218 -32.935 76.666 34.405 1.00 44.71 6 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 35.290 1.00 44.01 76.91 6 ATOM 66 N TRP B 219 -33.669 74.439 35.290 1.00 46.97 6											8
ATOM 39 O THR B 215											6
30 ATOM 40 N ASP B 216										1.00 52.51	
ATOM 41 CA ASP B 216	30									1.00 53.48	
ATOM 42 CB ASP B 216	-								40.829		
ATOM 43 CG ASP B 216 -36.674 74.005 41.650 1.00 70.57 6 ATOM 44 OD1 ASP B 216 -37.675 72.981 41.710 1.00 78.07 6 ATOM 45 OD2 ASP B 216 -38.228 72.588 40.652 1.00 82.31 8 ATOM 46 C ASP B 216 -37.983 72.567 42.830 1.00 86.55 8 ATOM 47 O ASP B 216 -35.920 75.123 39.648 1.00 58.42 6 ATOM 48 N GLU B 217 -34.954 75.979 39.984 1.00 56.85 8 ATOM 49 CA GLU B 217 -34.954 75.979 39.984 1.00 54.92 7 ATOM 50 CB GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 51 CG GLU B 217 -34.104 78.264 40.251 1.00 51.02 6 ATOM 52 CD GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 53 OEI GLU B 217 -34.089 80.443 41.945 1.00 40.00 6 ATOM 55 C GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 55 C GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 55 C GLU B 217 -34.851 77.612 37.018 1.00 53.55 6 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 60 CG GLU B 218 -30.965 75.793 36.981 1.00 40.86 6 ATOM 60 CG GLU B 218 -30.965 75.793 36.981 1.00 40.86 6 ATOM 61 CD GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 65 O GLU B 218 -32.318 76.159 38.072 1.00 39.88 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 66 CB TRP B 219 -33.669 74.439 35.290 1.00 46.07 6								73.865	40.435		
ATOM 44 OD1 ASP B 216									41.650		
ATOM 45 OD2 ASP B 216					ASP E	3 216			41.710		
ATOM 46 C ASP B 216	35			ODI	ASP E	3 216	-38.228	72.588			
ATOM 46 C ASP B 216	33						-37.983	72.567			
ATOM 48 N GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 50 CB GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 51 CG GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 52 CD GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 53 OEI GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 54 OE2 GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.815 77.612 37.018 1.00 53.55 6 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 59 CB GLU B 218 -32.318 76.385 36.981 1.00 49.20 7 ATOM 60 CG GLU B 218 -30.965 75.793 36.981 1.00 49.86 6 ATOM 61 CD GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 62 OEI GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6							-35.920				
ATOM 48 N GLU B 217 -34.954 75.979 39.984 1.00 54.92 7 40 ATOM 50 CB GLU B 217 -34.851 77.259 39.353 1.00 53.37 6 ATOM 51 CG GLU B 217 -34.104 78.264 40.251 1.00 51.02 6 ATOM 52 CD GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 53 OE1 GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 54 OE2 GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 55 C GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 56 O GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 58 CA GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 60 CG GLU B 218 -30.965 75.793 36.981 1.00 49.20 7 ATOM 61 CD GLU B 218 -30.965 75.793 36.981 1.00 49.86 6 ATOM 62 OE1 GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6							-36.847				
ATOM				N	GLU E	3 217	-34.954				
ATOM 50 CB GLU B 217 -34.104 78.264 40.251 1.00 51.02 6 ATOM 51 CG GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 52 CD GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 53 OE1 GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 54 OE2 GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.232 77.163 37.957 1.00 53.55 6 ATOM 56 O GLU B 217 -34.815 77.612 37.018 1.00 54.33 8 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 59 CB GLU B 218 -30.065 75.793 36.981 1.00 43.43 6 ATOM 61 CD GLU B 218 -30.065 76.728 37.801 1.00 43.43 6 ATOM 61 CD GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.01 8 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6	40			CA	GLU E	3 217					
ATOM 51 CG GLU B 217 -34.151 79.689 39.679 1.00 40.00 6 ATOM 52 CD GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 53 OE1 GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 54 OE2 GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.232 77.163 37.957 1.00 53.55 6 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 59 CB GLU B 218 -30.965 75.793 36.981 1.00 43.43 6 ATOM 60 CG GLU B 218 -30.065 76.728 37.801 1.00 40.86 6 ATOM 61 CD GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 62 OE1 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6	40			CB	GLU B	217					
ATOM 52 CD GLU B 217 -34.301 80.745 40.739 1.00 40.00 6 ATOM 53 OE1 GLU B 217 -34.089 80.443 41.945 1.00 40.00 8 ATOM 54 OE2 GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.232 77.163 37.957 1.00 53.55 6 ATOM 56 O GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 58 CA GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 59 CB GLU B 218 -30.965 75.793 36.981 1.00 43.43 6 ATOM 60 CG GLU B 218 -30.065 76.728 37.801 1.00 40.86 6 ATOM 61 CD GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6				CG	GLU B	217					
ATOM 53 OE1 GLU B 217			52	CD	GLU B	217					
ATOM 54 OE2 GLU B 217 -34.625 81.921 40.411 1.00 40.00 8 ATOM 55 C GLU B 217 -34.232 77.163 37.957 1.00 53.55 6 ATOM 56 O GLU B 217 -34.815 77.612 37.018 1.00 54.33 8 ATOM 57 N GLU B 218 -33.063 76.572 37.839 1.00 49.20 7 ATOM 59 CB GLU B 218 -32.318 76.385 36.608 1.00 45.94 6 ATOM 60 CG GLU B 218 -30.965 75.793 36.981 1.00 43.43 6 ATOM 61 CD GLU B 218 -30.065 76.728 37.801 1.00 40.86 6 ATOM 62 OE1 GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6			53	OE1							
ATOM 55 C GLU B 217		ATOM	54	OE2	GLU B	217					
ATOM 56 O GLU B 217	45	ATOM	55								
ATOM 57 N GLU B 218		ATOM									6
ATOM 58 CA GLU B 218		ATOM									8
ATOM 59 CB GLU B 218 -30.965 75.793 36.608 1.00 45.94 6 ATOM 60 CG GLU B 218 -30.065 76.728 37.801 1.00 40.86 6 ATOM 61 CD GLU B 218 -28.713 76.159 38.072 1.00 39.88 6 ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 64 C GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 65 O GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6											7
50 ATOM 60 CG GLU B 218										1.00 45.94	6
ATOM 61 CD GLU B 218	50								36.981		
ATOM 62 OE1 GLU B 218								76.728	37.801		
ATOM 63 OE2 GLU B 218 -28.606 74.967 38.449 1.00 37.61 8 ATOM 63 OE2 GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 65 O GLU B 218 -32.935 75.686 34.405 1.00 45.31 8 ATOM 67 CA TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6								76.159	38.072		
ATOM 63 GE2 GLU B 218 -27.707 76.901 37.945 1.00 34.01 8 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 65 O GLU B 218 -32.935 75.686 34.405 1.00 45.31 8 ATOM 67 CA TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6				OEI	GLU B	218	-28.606	74.967			
55 ATOM 64 C GLU B 218 -33.014 75.475 35.610 1.00 44.71 6 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6							-27.707	76.901			
ATOM 65 O GLU B 218 -32.935 75.686 34.405 1.00 45.31 8 ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6	5.5						-33.014				
ATOM 66 N TRP B 219 -33.669 74.439 36.131 1.00 44.02 7 ATOM 68 CB TRP B 219 -34.368 73.490 35.290 1.00 46.97 6	33										
ATOM 67 CA TRP B 219 -34.368 73.490 35.290 1.00 46.97 6				N	TRP B	219					
ATOM 68 CB TRR R 210 25 25 25 25 25 25 25 25 25 25 25 25 25				CA	TRP B	219					
72.400 30.119 1.00 48.42 6		ATOM	68								
								2.100	50.119	1.00 48.42	6

	*									- 3
5	ATOM	69		RP B		-34.195	71.230	36.374	1.00 54.61	6
	MOTA	70		RP B	219	-34.048	70.120	35.478	1.00 55.24	6
	ATOM	71			219	-33.076	69.248	36.063	1.00 53.67	6
	ATOM	72			219	-34.615	69.771	34.252	1.00 54.55	6
	ATOM	73	CD1 1	RP B	219	-33.399	71.019	37.415	1.00 55.75	6
10	MOTA	74	NE1 7	RP B	219	-32.697	69.838	37.236	1.00 54.43	7
	ATOM	75	CZ2 T	CRP B	219	-32.635	68.075	35.431	1.00 52.54	6
	ATOM	76	cz3 7	rrp B	219	-34.214	68.603	33.643	1.00 55.17	6
	ATOM	77	CH2	rrp B	219	-33.234	67.758	34.214	1.00 55.59	6
	ATOM	78	C :	TRP B	219	-35.409	74.199	34.459	1.00 47.32	6
15	ATOM	79		TRP B	219	-35.561	73.914	33.277	1.00 43.56	8
	MOTA	80		GLU B	220	-36.126	75.130	35.084	1.00 49.91	7
	ATOM	81		GLU B		-37.158	75.874	34.402	1.00 53.57	6
	ATOM	82		GLU B		-37.811	76.820	35.373	1.00 58.18	6
	ATOM	83		GLU B		-39.251	76.812	35.221	1.00 73.13	6
20	ATOM	84		GLU B		-39.824	76.858	36.489	1.00 80.06	6
20	ATOM	85		GLU B		-39.485	75.995	37.324	1.00 82.12	8
	ATOM	86		GLU B		-40.635	77.740	36.718	1.00 82.78	8
	ATOM	87		GLU E		-36.539	76.645	33.250	1.00 50.51	6
	MOTA	88		GLU E		-37.160	76.793	32.195	1.00 49.94	8
25	ATOM	89		LEU E		-35.312	77.135	33.455	1.00 43.71	7
23		90		LEU E		-34.604	77.884	32.411	1.00 42.81	6
	ATOM	91		LEU E		-33.214	78.324	32.865	1.00 39.21	6
	ATOM	92		LEU E		-32.321	78.833	31.754	1.00 36.34	6
	ATOM	93		LEU E	-	-33.073	79.843	30.927	1.00 36.93	6
20	ATOM	94		LEU E		-31.058	79.446	32.331	1.00 24.18	6
30	ATOM	95		LEU F		-34.454	77.011	31.192	1.00 43.46	6
	ATOM	96		LEU F		-34.819	77.406	30.104	1.00 45.25	8
	ATOM	97	N	ILE F	•	-33.878	75.829	31.398	1.00 39.09	7
	MOTA	98	CA		3 222	<u>-3</u> 3.687	74.857		1.00 35.47	6
25	ATOM	99	CB	ILE I		-33.224	73.516	30.871	1.00 33.74	6
35	MOTA	100	CG2	ILE !	•	-33.204	72.488	29.776	1.00 28.86	6
	MOTA	100	CG2	ILE I		-31.840	73.631	31.493	1.00 33.33	6
	ATOM		CD1		3 222	-31.435	72.419	32.264	1.00 34.85	6
	MOTA	102	CDI		B 222	-34.991	74.627	29.598	1.00 34.26	6
40	ATOM	103	0		B 222	-35.082	74.832	28.392	1.00 31.90	8
40	ATOM	104	N		B 223	-35.992	74.183	30.346	1.00 39.49	7
	ATOM	105 106	CA		B 223	-37.300			1.00 44.43	6
	ATOM				B 223	-38.351	73.876		1.00 50.81	6
	ATOM	107	CB		B 223	-39.693			1.00 62.51	6
	ATOM	108	CG		B 223	-40.795			1.00 72.22	6
45	ATOM	109	CD		•	-42.163			1.00 74.55	6
	ATOM	110	CE		B 223	-43.268	73.243			7
	ATOM	111	NZ		B 223	-37.648				6
	ATOM	112	С		B 223					8
	ATOM	113			B 223	-38.337				7
50	ATOM	114	N		B 224	-37.146				6
	ATOM	115			B 224	-37.353				6
	MOTA	116			B 224	-36.956				8
	MOTA	117			B 224	-37.646				6
	MOTA	118			B 224	-37.273				6
55	ATOM	119			B 224	-36.521				
	ATOM	120			B 224	-37.043				8
	MOTA	121			B 225	-35.231				7
	ATOM	122	CA	VAL	B 225	-34.263	77.295	25.801	1.00 38.12	6

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5	ATOM	123	CE	VAL	B 225	-32.869	77.015	36 340		
	ATOM	124			B 225		_			6
	MOTA	125			B 225			-		6
	ATOM	126			B 225					6
	ATOM	127			B 225					6
10	ATOM	128			B 226					8
	ATOM	129			B 226			_		7
	ATOM	130			B 226				• • •	6
	ATOM	131			B 226					6
	ATOM	132			B 226	-36.413				8
15	ATOM	133			B 226	-36.664				6
	ATOM	134			B 226	-36.633	74.170	-		6
	ATOM	135			B 227		74.054	22.578		8
	ATOM	136			B 227	-37.746	74.542	24.480		7
	ATOM	137			B 227	-39.008	74.861	23.822	1.00 36.93	6
20	ATOM	138			B 227	-39.914	75.631	24.785	1.00 38.06	6
	ATOM	139			B 227	-38.686	75.719	22.608	1.00 37.69	6
	ATOM	140			B 228	-39.317	75.616	21.566	1.00 40.94	8
	ATOM	141	CA		B 228	-37.677	76.572	22.785	1.00 32.86	7
	ATOM	142	CB		B 228	-37.216	77.483	21.753	1.00 32.48	6
25	ATOM	143	С		B 228	-36.252	78.458	22.358	1.00 28.25	6
	ATOM	144	0			-36.545	76.704	20.638	1.00 36.12	6
	ATOM	145	N		B 228 B 229	-37.078	76.586	19.544	1.00 37.86	8
	ATOM	146	CA			-35.364	76.175	20.924	1.00 33.58	7
	ATOM	147	CB		B 229 B 229	-34.611	75.409	19.956	1.00 32.97	6
30	ATOM	148	CG		B 229	-33.418	74.721	20.597	1.00 33.69	6
	ATOM	149		HIS		-32.776	73.714	19.715	1.00 28.39	6
	ATOM	150		HIS		-32.535	72.384	19.863	1.00 28.83	6
	ATOM	151		HIS		-32.336	74.030	18.426	1.00 30.47	7
	ATOM	152		HIS		-31.867	72.929	17.855	1.00 26.95	6
35	ATOM	153	C		B 229	-31.976	71.927	18.700	1.00 31.27	7
	ATOM	154	0		B 229	-35.362	74.352	19.202	1.00 38.40	6
	ATOM	155	N		B 229	-35.069	74.131	18.045	1.00 41.49	8
	ATOM	156	CA		B 230	-36.296	73.688	19.882	1.00 38.55	7
	ATOM	157	CB		B 230	-37.077	72.634	19.263	1.00 40.40	6
40	ATOM	158		VAL 1		-37.744	71.747	20.310	1.00 44.68	6
	ATOM	159		VAL I		-38.381	70.537	19.637	1.00 39.39	6
	ATOM	160	CGZ			-36.742	71.311	21.356	1.00 42.18	6
	ATOM	161	0	VAL		-38.133	73.130	18.284	1.00 44.28	6
	ATOM	162	N		3 230	-38.375	72.505	17.248	1.00 45.94	8
45	ATOM	163	CA	ALA E		-38.774	74.240	18.623	1.00 45.59	7
-	ATOM	164	CB	ALA E		-39.820	74.804	17.792	1.00 47.84	6
	ATOM	165	СВ	ALA E		-40.736	75.661	18.647	1.00 45.08	6
	ATOM	166		ALA E		-39.235	75 .6 36	16.673	1.00 48.04	6
	ATOM	167	0	ALA E		-39.959	76.128	15.816	1.00 49.95	8
50	ATOM	168	N	THR E		-37.914	75.773	16.669	1.00 47.26	7
30	ATOM		CA	THR E		-37.220	76.563	15.654	1.00 43.64	6
	ATOM	169	CB	THR E		-36.482	77.746	16.315	1.00 41.93	6
		170	OG1			-35.385	77.270	17.098	1.00 39.10	8
	ATOM	171	CG2			-37.423	78.523	17.232	1.00 29.80	6
55	ATOM	172	С	THR B		-36.194	75.719	14.914	1.00 43.97	6
23	ATOM	173	0	THR B		-35.401	76.252	14.155	1.00 40.55	8
	ATOM	174	N	ASN B		-36.195	74.407	15.157	1.00 48.62	7
	ATOM	175	CA	ASN B		-35.247	73.511	14.483	1.00 58.62	6
	ATOM	176	CB	ASN B	233	-34.621	72.537	15.500	1.00 62.44	6
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5	ATOM	177	CG	ASN B		-33.4		71.812	14.946		68.35	6
	ATOM	178		ASN B		-32.5		72.427	14.256		65.50	8
	ATOM	179	ND2	ASN B		-33.2		70.529	15.265		74.29	7 6
	MOTA	180	С		233	-36.0		72.755	13.437		65.06	8
	ATOM	181	0	ASN B		-36.9		72.005	13.754		69.47	7
10	MCTA	182	N	ALA B		-35.6		72.986	12.182		68.80	6
	ATOM	183	CA	ALA B		-36.3		72.376	11.036		70.98	6
	MOTA	184	CB	ALA B		-35.5		72.701	9.769		71.43	6
	MOTA	185	С	ALA B		-36.5		70.880	11.111		73.83	8
	MOTA	186	0	ALA B		-35.0		70.142	11.50		74.33 75.07	7
15	MOTA	187	N	GLN B		-37.		70.479	10.717		76.32	6
	MOTA	188	CA	GLN B		-38.		69.095	10.690		76.32	6
	MOTA	189	CB	GLN B		-37.		68.365	9.533		77.07	6
	MOTA	190	CG	GLN B		-38.		68.540	8.170		80.85	6
	MOTA	191	CD	GLN E		-38.		69.940	7.909		82.01	8
20	MOTA	192	OE1			-39.		70.401	8.49		78.80	7
	ATOM	193	NE2			-37.		70.620	7.04		77.15	6
	MOTA	194	С	GLN E		-37.		68.331	11.95			8
	MOTA	195	0	GLN E		-38.		67.137	11.94° 13.03			7
	MOTA	196	N	GLY E		-37.		68.985	14.28		78.37	6
25	MOTA	197	CA	GLY F		-37.		68.263	14.21		79.43	6
	MOTA	198	С	GLY i		-36.		66.882	13.54			8
	ATOM	199	0	GLY I		-35.		66.650	14.94			7
	ATOM	200	N	SER I		-37.		66.007 64.600	15.09			6
	ATOM	201	CA	SER I		-37. -38.		63.953	16.06		76.46	6
30	ATOM	202	CB	SER I		-30. -37.		63.895	13.73		75.35	6
	ATOM	203	С		B 237 B 237	-37. -36.		62.911	13.52			8
	ATOM	204	0		B 238	-38.		64.443	12.84			7
	MOTA	205 206	N CA		B 238		293	63.926	11.51			6
35	ATOM— ATOM	207	CB		B 238		663	64.397	11.09	6 1.00	75.85	6
33	ATOM	208	C		B 238		.369	64.216	10.38		74.10	67
	ATOM	209	0		B 238		.747	64.135	9.22		75.34	8
	ATOM	210	N		в 239	-36	.127	64.427	10.65		73.39	7
	ATOM	211	CA		B 239	-35	.345	64.786	9.51		74.02	6
40	ATOM	212	СВ		B 239	-34	.121	65.542	9.93			6
	ATOM	213			в 239	-33	.085	64.786	10.73		0 89.67	6
	ATOM	214		2 TRP	B 239	-31	.727	64.530			0 93.19	6
	ATOM	215		2 TRP		-31	.069	63.848	11.39		0 95.46	6
	ATOM	216		3 TRP	B 239	-30	.949	64.941			0 95.35	6
45	ATOM	217	CD	1 TRP	B 239	-33	.237	64.180			0 94.16	6
	ATOM	218	NE	1 TRP	B 239		.022	63.631			0 97.48	7
	ATOM	219	CZ	2 TRP	B 239	-29	.706				0 96.23	6
	ATOM	220	CZ	3 TRP	B 239		.613				0 96.75	6
	ATOM	221	. CH	2 TRP	в 239	-28	.978				0 97.32	6
50	ATOM	222	. C	TRP	в 239		.994				0 70.77	
	ATOM	223	0		B 239		.423				0 71.70	
	MOTA	224	N	LYS	B 240		.165				0 67.10	
	ATOM	225	CP	LYS	B 240		.724				0 65.63	
	ATOM	226	CE		B 240		.321				0 66.65	
55		227	Co		B 240		.210				0 69.83	
	ATOM	228			B 240		.759				0 71.49	
	ATOM	229			B 240		.576				0 71.31 0 72.23	
	MOTA	230) N2	LYS	B 240	-30	.106	58.604	12.1	J/ 1.0	12.23	,

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5	ATOM	231		LYS	B 240	-34.719	61.331	6.996	1.00 66.19	6
	ATOM	232	0	LYS	B 240	-34.321		6.031		8
	ATOM	233	N	ASN	B 241	-35.986		7.139		7
	ATOM	234	CA	ASN	B 241	-37.031		6.171		6
	MOTA	235	CB	ASN	B 241	-38.240		6.915		6
10	ATOM	236	CG	ASN :	B 241	-37.966		7.544		
	MOTA	237	ODI		B 241	-37.561		6.845		6
	ATOM	238			B 241	-38.205		8.836		8
	ATOM	239			B 241	-37.496		5.255		7
	ATOM	240	0		B 241	-38.504	62.395	4.578	1.00 64.76	6
15	ATOM	241	N		B 242	-36.753		5.209	1.00 64.76	8
	ATOM	242	CA		B 242	-37.096		4.362	1.00 67.46	7
	ATOM	243	СВ		B 242	-37.501	65.948	5.258	1.00 67.46	6
	ATOM	244	CG		3 242	-38.746	65.684	6.076		6
	ATOM	245	CD	LYS I		-40.007	65.528	5.215		6
20	ATOM	246	CE	LYS I		-40.416	66.852	4.564	1.00 74.32 1.00 74.41	6
	ATOM	247	NZ	LYS I		-40.657	67.941	5.575	1.00 74.41	6
	ATOM	248	С	LYS I		-35.826	65.081	3.592		7
	ATOM	249	0	LYS E		-35.814	65.799	2.601	1.00 66.28	6
	ATOM	250	N	ARG I		-34.763	64.485	4.112	1.00 67.61	8
25	MOTA	251	CA	ARG E		-33.410	64.577	3.591	1.00 64.19 1.00 62.43	7
	ATOM	252	СВ	ARG E		-32.599	63.547	4.390	1.00 62.43	6
	ATOM	253	CG	ARG E		-31.128	63.558	4.171	1.00 60.12	6
	ATOM	254	CD	ARG E	,	-30.335	62.888	5.319	1.00 40.00	6
	MOTA	255	NE	ARG E		-30.269	61.428	5.296	1.00 40.00	6 7
30	ATOM	256	CZ	ARG E		-29.384	60.724	6.009	1.00 40.00	6
	MOTA	257	NH1			-28.510	61.357	6.798	1.00 40.00	7
	MOTA	258	NH2	ARG E	243	-29.355	59.401	5.908	1.00 40.00	7
	ATOM	259	С	ARG E	243	-33.408	64.252	2.100	1.00 40.00	6
	ATOM	260	0	ARG E	243	-33.690	63.122	1.722	1.00 63.96	8
35	ATOM	261	N	LYS E	244	-33.105	65.245	1.270	1.00 62.41	7
	ATOM	262	CA	LYS E	244	-33.054	65.053	-0.179	1.00 61.57	6
	MOTA	263	CB	LYS B	244	-34.104	65.941	-0.866	1.00 63.68	6
	ATOM	264	CG	LYS B	244	-35.527	65.731	-0.337	1.00 71.29	6
	MOTA	265	CD	LYS B	244	-36.566	66.549	-1.107	1.00 73.83	6
40	MOTA	266	CE	LYS B	244	-36.219	68.045	-1.138	1.00 74.71	6
	ATOM	267	NZ	LYS B		-36.169	68.689	0.219	1.00 73.32	7
	MOTA	268	С	LYS B	244	-31.658	65.402	-0.670	1.00 59.30	6
	ATOM	269	0	LYS B	244	-31.317	66.570	-0.852	1.00 56.34	8
	ATOM	270	N	PHE B		-30.858	64.359	-0.875	1.00 57.06	7
45	ATOM	271	CA	PHE B		-29.462	64.525	-1.305	1.00 59.01	6
	ATOM	272	CB	PHE B		-28.786	63.179	-1.478	1.00 59.62	6
	MOTA	273	CG	PHE B		-28.991	62.288	-0.339	1.00 66.60	6
	MOTA	274		PHE B		-30.200	61.669	-0.172	1.00 67.17	6
	MOTA	275		PHE B		-28.012	62.117	0.593	1.00 69.25	6
50	ATOM	276		PHE B		-30.404	60.882	0.911	1.00 69.92	6
	ATOM	277		PHE B	245	-28.229	61.329	1.669	1.00 70.50	6
	ATOM	278	CZ	PHE B	245	-29.418	60.714	1.830	1.00 70.89	6
	ATOM	279	С	PHE B	245	-29.301	65.282	-2.592	1.00 60.68	6
	ATOM	280	0	PHE B	245	-29.859	64.911	-3.619	1.00 62.37	8
55	ATOM	281	N	LEU B	246	-28.495	66.336	-2.505	1.00 62.37	7
	MOTA	282	CA	LEU B	246	-28.201	67.199	-3.631	1.00 59.44	6
	ATOM	283	СВ	LEU B	246	-27.248	68.332	-3.231	1.00 57.43	6
	ATOM	284		LEU B		-27.118	69.474	-4.207	1.00 54.41	6
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                                                          -6.363
             290
                       PRO B 247
                                       -28.839
10
    ATOM
                   CD
                                                                   1.00 63.56
                                                                                  6
                                       -27.391
                                                 65.958
                                                          -7.130
             291
                   CA
                       PRO B 247
     ATOM
                                                                    1.00 64.42
                                                                                  6
                                                 66.675
                                                          -8.340
                       PRO B 247
                                       -27.976
             292
                   CB
    ATOM
                                                                    1.00 64.90
                                                                                  6
                       PRO B 247
                                       -28.873
                                                 67.714
                                                           -7.841
             293
                   CG
     ATOM
                                                           -7.143
                                                                    1.00 61.94
                                                                                  6
                                                 65.947
                                       -25.866
                        PRO B 247
     MOTA
             294
                   С
                                                                                  8
                                                                    1.00 61.60
                                                  66.944
                                                           -6.856
                                       -25.223
             295
                   0
                        PRO B 247
15
     MOTA
                                                                                  7
                                                           -7.478
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                                                  64.771
                        GLU B 248
                                       -25.333
             296
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     MOTA
                                                                    1.00 63.50
                                                                                  6
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                                       -23.896
                                                  64.516
     ATOM
              297
                   CA
                        GLU B 248
                                                                                   6
                                                           -8.248
                                                                    1.00 66.94
                                       -23.630
                                                  63.154
              298
                   CB
                        GLU B 248
     MOTA
                                                                    1.00 68.70
                                                                                   6
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                                                  62.953
                                                           -8.713
              299
                   CG
                        GLU B 248
     MOTA
                                                  61.745
                                                           -9.580
                                                                    1.00 40.00
                                                                                   6
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20
     ATOM
              300
                   CD
                        GLU B 248
                                                                    1.00 40.00
                                                                                   8
                                                  61.007 -10.035
                                        -22.863
              301
                   OE1 GLU B 248
     ATOM
                                                                    1.00 40.00
                                                                                   8
                                                  61.460
                                                           -9.838
                                        -20.709
              302
                   OE2 GLU B 248
     ATOM
                                                                                   6
                                        -23.158
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                                                           -8.415
                                                                    1.00 64.19
                        GLU B 248
     MOTA
              303
                   С
                                                  65.975
                                                           -8.066
                                                                    1.00 65.56
                                                                                   8
              304
                   0
                        GLU B 248
                                        -22.056
     MOTA
                                                                                   7
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                                        -23.796
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                        ASP B 249
25
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     MOTA
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                                                                                   6
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                   CA
                                                                    1.00 62.97
                                                                                   6
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              307
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                        ASP B 249
     MOTA
                                                  67.715 -11.489
                                                                    1.00 64.63
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              308
                        ASP B 249
                                        -25.437
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                                                                                   8
                                                                    1.00 64.84
                                                  67.285 -10.629
                                        -26.235
              309
                   OD1 ASP B 249
     MOTA
                                                  68.718 -12.189
                                                                    1.00 66.52
                                                                                   8
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30
     ATOM
              310
                    OD2 ASP B 249
                                                                                   6
                                                  68.413
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                                                                    1.00 64.31
                                        -23.068
              311
                    С
                        ASP B 249
     ATOM
                                                  69.084 -10.355
                                                                    1.00 64.73
                                                                                   8
                                        -22.117
                        ASP B 249
     MOTA
              312
                    0
                                                                    1.00 63.09
                                                                                   7
                                                  68.892
                                                           -9.136
                                        -23.987
              313
                    N
                        ILE B 250
     MOTA
                                        -23.921
                                                           -8.660
                                                                    1.00 64.39
                                                                                   6
                                                  70.281
     MOTA
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                    CA
                        ILE B 250
                                                                                   6
                                                           -7.798
                                                                    1.00 65.79
                                                  70.575
35
              315
                    CB
                        ILE B 250
                                        -25.124
     MOTA
                                                                                   6
                                                                    1.00 64.78
                                                  72.041
                                                           -7.858
                    CG2 ILE B 250
                                        -25.559
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     MOTA
                                                                                   6
                                                           -8.206
                                                                    1.00 65.28
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                    CG1 ILE B 250
     MOTA
              317
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                                                           -7.887
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                    CD1 ILE B 250
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              318
     MOTA
                                                           -7.714
                                                                     1.00 65.21
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                        ILE B 250
                                        -22.815
     MOTA
              319
                    С
                                                                                   8
                                                  69.847
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                                                                     1.00 64.05
                                        -22.754
                        ILE B 250
 40
     MOTA
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                    0
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                                                           -8.103
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                                                  71.392
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                    N
                        GLY B 251
                                                                     1.00 67.32
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                                                  71.721
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              322
                    CA
      ATOM
                                                                     1.00 68.52
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                                                  70.806
                        GLY B 251
      MOTA
              323
                    C
                                                                                   8
                        GLY B 251
                                                  70.548
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                                                                     1.00 65.49
                                        -19.791
              324
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      MOTA
                                                                                   7
                                                           -6.799
                                                                     1.00 72.26
                                                  70.440
 45
                         GLN B 252
                                        -19.074
      MOTA
              325
                    Ν
                                                                     1.00 74.10
                                                                                   6
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                                                           -6.883
                                        -17.949
                         GLN B 252
      MOTA
              326
                    CA
                                                                     1.00 75.82
                                                                                   6
                                                           -6.723
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      MOTA
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                    CB
                         GLN B 252
                                        -18.460
                                                                                   6
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                                                           -6.356
                         GLN B 252
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                                                   67.088
              328
                    CG
      MOTA
                                                                     1.00 79.38
                                                                                   6
                                                   65.759
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                                        -17.924
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                    CD
                         GLN B 252
      ATOM
                                                                     1.00 80.55
                                                            -6.549
                                                                                   8
                                                   65.042
                    OE1 GLN B 252
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 50
      ATOM
               330
                                                                     1.00 78.12
                                                                                   7
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                                        -17.661
                                                   65.380
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                    NE2 GLN B 252
      MOTA
                                                   69.727
                                                           -8.258
                                                                     1.00 77.17
                                                                                    6
                         GLN B 252
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               332
                    С
                                                                     1.00 76.50
                                                                                   8
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                         GLN B 252
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                                                   70.009
                    0
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                                                                                   7
                                                           -8.279
                                                                     1.00 80.78
                                                   69.795
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                    N
                         ALA B 253
      ATOM
                                                                     1.00 83.70
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                    CA
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                                        -14.615
 55
      ATOM
               335
                         ALA B 253
                                                                     1.00 83.23
                                                                                    6
                                                   70.914
                                                            -7.255
               336
                    CB
                         ALA B 253
                                        -13.794
      MOTA
                                                                     1.00 85.59
                                                            -9.731
                                                                                    6
                                        -13.605
                                                   70.732
               337
                    С
                         ALA B 253
      MOTA
                                                   69.691 -10.171
                                                                     1.00 85.69
                                                                                    8
                                        -13.186
               338
                    0
                         ALA B 253
      ATOM
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5	ATOM	339			B 254	-13.223	71.944	-10.246	1.00 35.05	7
	ATOM	340			B 254	-13.798		-9.752		6
	ATOM	341			B 254	-12.266		-11.351	1.00 35.89	6
	ATOM	342			B 254	-12.275	73.710	-11.596	1.00 33.94	6
10	ATOM	343			B 254	-13.222	74.277	-10.688	1.00 33.31	6
10	ATOM	344	С		B 254	-10.827	71.665	-11.121	1.00 37.75	6
	ATOM	345	0	PRO 1	3 254	-10.379	71.426	-10.009	1.00 38.78	8
	TER	_								
	ATOM	1	N	GLY I		-8.238	79.356	-2.979	1.00 40.00	7
1.5	ATOM	2		GLY I		-9.314	78.411	-3.005	1.00 40.00	6
15	ATOM	3	С	GLY I		-10.206	78.717	-4.355	1.00 40.00	6
	ATOM	4	0	GLY I		-11.372	79.141	-4.256	1.00 40.00	8
	MOTA	5	N	GLY E		-9.565	78.527	-5.597	1.00 40.00	7
	ATOM	6	CA	GLY E		-10.136	78.609	-7.087	1.00 40.00	6
20	ATOM	7	С	GLY E		-10.849	79.966	-7.577	1.00 40.00	6
20	ATOM	8	0	GLY E		-10.200	81.044	-7.543	1.00 40.00	8
	ATOM	9	N	LYS E		-12.086	79.687	-8.124	1.00 61.71	7
	ATOM	10	CA	LYS E		-13.323	80.536	-8.428	1.00 64.36	6
	ATOM	11	С	LYS E		-14.367	79.750	-7.614	1.00 63.41	6
26	ATOM	12	0	LYS E		-14.102	78.579	-7.280	1.00 61.93	8
25	ATOM	13	CB	LYS E		-13.901	80.405	-9.876	1.00 63.50	6
	ATOM	14	CG	LYS E		-13.487	81.474	-10.881	1.00 20.00	6
	ATOM	15	CD	LYS Ē		-14.016		-10.612	1.00 20.00	6
	ATOM	16	CE	LYS E		-13.641	83.874	-11.742	1.00 20.00	6
20	ATOM	17	NZ	LYS E		-13.680	85.287	-11.341	1.00 20.00	7
30	ATOM	18	N	VAL E		-15.489	80.335	-7.307	1.00 61.15	7
•	ATOM	19	CA	VAL B	• • •	-16.616	79.632	-6.619	1.00 59.46	6
	ATOM	20	CB	VAL B		-17.574	80.703	-6.099	1.00 59.03	6
	ATOM	21	CG1			-18.479	80.215	-4.979	1.00 53.79	6
35	ATOM	22	CG2			-16.847	81.938	-5.562	1.00 55.32	6
33	ATOM	23	С	VAL B		-17.330	78.824	-7.700	1.00 60.96	6
	ATOM	24	0	VAL B		-16.940	78.873	-8.873	1.00 62.13	8
	ATOM	25	N	ASP B		-18.378	78.098	-7.340	1.00 62.59	7
	ATOM ATOM	26	CA	ASP B		-19.175	77.339	-8.312	1.00 64.95	6
40		27	CB	ASP B		-18.796	75.851	-8.270	1.00.64.32	6
70	ATOM ATOM	28	CG	ASP B		-19.928	75.022	-8.584	1.00 67.70	6
	ATOM	29		ASP B		-20.856	75.062	-9.295	1.00 72.59	8
	ATOM	30 31		ASP B		-20.370	73.959	-8.310	1.00 68.84	8
	ATOM	32	С	ASP B	•	-20.658	77.614	-8.016	1.00 65.64	6
45	ATOM	33	O N	ASP B		-21.342	76.895	-7.313	1.00 68.81	8
15	ATOM	34	N	LEU B		-21.066	78.737	-8.588	1.00 65.12	7
	ATOM	35	CA	LEU B		-22.385	79.330	-8.499	1.00 63.40	6
	ATOM	36	CB	LEU B		-22.429	80.448	-9.542	1.00 67.34	6
	ATOM	37	CG	LEU B		-21.295	81.459	-9.399	1.00 69.35	6
50	ATOM	38		LEU B		-20.983	82.127		1.00 68.24	6
50	ATOM	39	CD2	LEU B		-21.663	82.461	-8.344	1.00 70.47	6
	ATOM	40		LEU B		-23.673	78.507	-8.602	1.00 59.67	6
	ATOM		0	LEU B		-24.684	78.890	-7.988	1.00 53.35	8
	ATOM	41	N	GLU B		-23.677	77.416	-9.371	1.00 58.01	7
55	ATOM	42	CA	GLU B		-24.901	76.640	-9.449	1.00 58.34	6
,,	ATOM	43	CB	GLU B		-24.752	75.410 -		1.00 59.21	6
		44	CG	GLU B		-25.979	74.464 -		1.00 62.89	6
	ATOM	45	CD	GLU B		-26.048	73.419 -		1.00 67.66	6
	ATOM	46	OEI	GLU B	261	-25.076	72.645 -	-11.512	1.00 69.95	8

5	ATOM	47	OE2 G	LU B	267	-27.098	73.328		1.00		8
	MOTA	48		LU B		-25.200	76.184	-8.032	1.00		6
	MOTA	49		LU B		-26.354	76.009	-7.643	1.00		8
	ATOM	50		LA B		-24.114	75.996	-7.285	1.00		7
	ATOM	51		LA B		-24.151	75.560	-5.905	1.00		6
10	ATOM	52		LA B		-22.816	74.956	-5.526	1.00		6
	ATOM	53		LA B		-24.421	76.775	-5.056	1.00		6
	MOTA	54		LA B		-25.419	76.823	-4.351	1.00		8
	ATOM	55			269	-23.533	77.766	-5.142	1.00		7
	MOTA	56	CA F		269	-23.688	78.989	-4.358		43.96	6
15	MOTA	57	CB F		269	-22.903	80.150	-4.971		40.10	6
	ATOM	58			269	-23.057	81.458	-4.224		40.44	6
	ATOM	59	CD1 E			-22.284	81.727	-3.105		38.98	6
	ATOM	60			269	-24.033	82.372	-4.603		37.15	6
	ATOM	61		PHE B		-22.472	82.921	-2.388		32.12	6
20	MOTA	62		PHE B		-24.228	83.567	-3.890		38.41	6
	MOTA	63		PHE B		-23.457	83.838	-2.780		40.55	6
	ATOM	64		PHE B		-25.154	79.374	-4.320		49.76	6
	MOTA	65		PHE E		-25.645	79.905	-3.336		52.15	8
	MOTA	66		SER É		-25.840	79.112	-5.426		53.15	7
25	ATOM	67		SER E		-27.253	79.431	-5.520		52.29	6
	ATOM	68		SER E		-27.742	79.274	-6.948		51.85	6
	MOTA	69		SER E	-	-29.118	79.606	-7.048		53.42	8 6
	MOTA	70		SER E		-28.012	78.486	-4.630		49.38	8
	ATOM	71			3 270	-28.438	78.864	-3.548		48.74	7
30	ATOM	72		HIS E		-28.185	77.253	-5.115		50.15 51.67	6
	MOTA	73			3 271	-28.904	76.203	-4.382		58.52	6
	MOTA	74			3 271	-28.409		-4.782 -5.976		68.97	6
	ATOM	75			3 271	-29.096		-6.102		70.88	6
	ATOM	76			3 271	-29.987	73.233 74.770	-7.270		71.98	7
35	ATOM	77			3 271	-28.943		-8.100		73.91	6
	ATOM	78			B 271	-29.716 -30.354	_	-7.419		73.59	7
	MOTA	79			B 271 B 271	-28.785		-2.886		48.33	6
	ATOM	80				-29.641		-2.156		48.39	8
40	ATOM	81			B 271	-27.702		-2.444		41.34	7
40	ATOM	82	N GP		В 272 В 272	-27.440		-1.033		39.44	6
	ATOM	83	CA		•	-25.936				36.67	6
	ATOM	84	CB CG		В 272 В 272	-25.241				33.39	6
	ATOM	85 86			B 272	-23.856				33.14	6
45	ATOM ATOM	87			B 272	-25.973				38.28	6
43	MOTA	88			B 272	-23.200				38.26	6
	ATOM	89			B 272	-25.321				43.28	6
	MOTA	90	CZ		B 272	-23.937				39.74	6
	ATOM	91	C		B 272	-28.144				40.75	6
50	ATOM	92	0		B 2.72	-28.803				35.51	8
30	ATOM	93	N		B 273	-28.027				41.64	7
	ATOM	94	CA		B 273	-28.658				45.97	6
			CB		B 273	-28.023				51.52	6
	ATOM	95 96			B 273	-28.292				45.74	8
55	ATOM ATOM	97			B 273	-26.51				49.73	6
23	ATOM	98	C		B 273	-30.142				46.23	6
	ATOM	99	0		B 273	-30.862				41.21	8
	ATOM	100			B 274	-30.583				46.21	7
	AIOM	100	14	فيب		23.30	_ ,_,_,				

5	ATOM	101	CA	LYS	В	274	-31.983	79.774	-2.147	1.00	54.53	6
	ATOM	102	CB	LYS	В	274	-32.133	78. 7 24	-3.232	1.00	54.36	6
	ATOM	103	С	LYS	В	274	-32.819	79.396	-0.931	1.00	56.88	· 6
	ATOM	104	0	LYS	В	274	-34.025	79.624	-0.906	1.00	57.98	8
	ATOM	105	N	ILE	В	275	-32.151	78.820	0.076	1.00	56.48	7
10	ATOM	106	CA	ILE	В	275	-32.791	78.381	1.332	1.00	52.64	6
	ATOM	107	СВ	ILE	В	275	-32.638	76.863	1.519	1.00	49.15	6
	ATOM	108	CG2	ILE	В	275	-33.505	76.105	0.529	1.00	47.42	6
	ATOM	109	CG1	ILE	В	275	-31.188	76.441	1.343	1.00	45.31	6
	ATOM	110	CD1	ILE	В	275	-30.990	74.952	1.391	1.00	37.22	6
15	ATOM	111	С	ILE	В	275	-32.241	79.086	2.574		51.78	6
	ATOM	112	0	ILE	В	275	-32.858	79.049	3.622		49.80	8
	ATOM	113	N	ILE	В	276	-31.071	79.709	2.435	1.00	51.76	7
	ATOM	114	CA			276	-30.410	80.409	3.533		52.58	6
	ATOM	115	СВ			276	-29.145	81.110	3.042		55.04	6
20	ATOM	116	CG2			276	-29.486	82.172	2.017		53.28	6
	ATOM	117	CG1			276	-28.396	81.786	4.203		57.31	6
	ATOM	118	CD1	ILE	В	276	-27.862	80.854	5.231		60.32	6
	MOTA	119	С			276	-31.282	81.461	4.237		50.70	6
	ATOM	120	0	ILE	В	276	-31.015	81.817	5.385		55.55	8
25	ATOM	121	N			277	-32.322	81.953	3.568	1.00	47.33	7
	ATOM	122	CA	THR	В	277	-33.174	82.968	4.141		42.59	6
	ATOM	123	СВ	THR	В	277	-34.042	83.632	3.048	1.00	44.97	6
	ATOM	124	OG1	THR	В	277	-33.202	84.145	2.001	1.00	46.38	8
	ATOM	125	CG2	THR	B	277	-34.856	84.781	3.653	1.00	37.17	6
30	ATOM	126	С	THR	В	277	-34.069	82.447	5.267	1.00	39.84	6
	ATOM	127	0	THR	В	277	-34.083	83.026	6.375	1.00	40.55	8
	ATOM	128	N	PRO	В	278	-34.832	81.385	5.017	1.00	38.20	7
	MOTA	129	CD	PRO	В	278	-34.925	80.666	3.747	1.00	36.34	6
	MOTA	130	CA	PRO	В	278	-35.711	80.834	6.059	1.00	36.63	6
35	MOTA	131	СВ	PRO	В	278	-36.475	79.715	5.357	1.00	32.95	6
	MOTA	132	CG	PRO	В		-35.833	79.516	4.056	1.00	35.75	6
	MOTA	133	С	PRO	В	278	-34.892	80.324	7.220	1.00	38.60	6
	ATOM	134	0	PRO			-35.372	80.157	8.331		37.67	8
	MOTA	135	N	ALA			-33.636	80.040	6.927		37.05	7
40	ATOM	136	CA			279	-32.696	79.525	7.903		33.18	6
•	ATOM	137	CB			279	-31.391	79.195	7.205		30.56	6
	MOTA	138	С			279	-32.447		8.991		33.47	6
	ATOM	139	0			279	-32.623	80.238	10.158		33.74	8
	ATOM	140	N			280	-32.010	81.728	8.577		29.96	7
45	MOTA	141	CA			280	-31.728	82.809	9.501		25.94	6
	ATOM	142	CB			280	-31.190	84.040	8.754		26.95	6
	ATOM	143		ILE			-30.881	85.149	9.715		15.40	6
	MOTA	144		ILE			-29.904	83.696	8.007		26.73	6
	MOTA	145	CDI	ILE			-29.255	84.878	7.362		34.31	6
50	MOTA	146	С			280	-32.964	83.172	10.310		31.39	6
	ATOM	147	0			280	-32.882	83.378	11.522		35.69	8
	ATOM	148	N	THR	В	281	-34.113	83.233	9.647	1.00	30.90	7
	ATOM	149	CA			281	-35.361	83.586	10.328		33.49	6
	MOTA	150	CB			281	-36.598	83.396	9.419		37.18	6
55	ATOM	151	OG1			281	-36.703	82.034	9.005		46.48	8
	ATOM	152	CG2			281	-36.525	84.289	8.198		32.85	6
	ATOM	153	С			281	-35.523	82.706	11.556		29.94	6
	ATOM	154	0	THR	В	281	-35.855	83.186	12.634	1.00	25.55	8

5	ATOM	155	N	ARG	В	282	-35.296	81.405	11.378	1.00	32.70	7
	ATOM	156	CA	ARG	В	282	-35.439	80.449	12.475		34.27	6
	ATOM	157	CB	ARG	В	282	-34.999	79.060	12.020		33.78	6
	ATOM	158	CG	ARG	В	282	-35.986	77.944	12.280		45.15	6
	ATOM	159	CD			282	-36.701	77.514	11.015		58.24	6
10	ATOM	160	NE			282	-35.771	77.153	9.969		68.41	7
	ATOM	161	CZ	ARG		282	-34.862	76.200	10.098		72.31	6
	ATOM	162	NH1	ARG		282	-34.779	75.502	11.232		77.89	7
	ATOM	163	NH2	ARG			-34.022	75.963	9.096		69.25	7
	ATOM	164	С			282	-34.556	80.919	13.622		34.81	6
15	ATOM	165	0			282	-35.008	81.034	14.753			
	ATOM	166	N			283	-33.288	81.183	13.289		36.03 31.71	8 7
	ATOM	167	CA			283	-32.304	81.667				
	ATOM	168	СВ			283	-30.993		14.249		30.16	6
	ATOM	169	CG1	VAL			-30.993	82.029	13.559		29.00	6
20	ATOM	170	CG2	VAL			-30.385	82.617	14.557		28.64	6
_0	ATOM	171	C	VAL				80.816	12.915		28.28	6
	ATOM	172	0	VAL			-32.848	82.884	14.994		32.50	6
	ATOM	173	N	VAL			-32.619	83.057	16.185		33.48	8
	ATOM	174	CA	VAL			-33.573	83.728	14.265		30.96	7
25	ATOM	175	CB	VAL			-34.177	84.925	14.844		29.14	6
	ATOM	176	CG1	VAL			-34.672	85.892	13.751		31.27	6
	ATOM	177	CG2	VAL			-35.278	87.129	14.371		24.21	6
	ATOM	178	C	VAL			-33.554	86.270	12.812		30.51	6
	ATOM	179	0	VAL			-35.336	84.498	15.747		28.89	6
30	ATOM	180	N	ASP			-35.491	84.994	16.860		27.29	8
50	ATOM	181	CA	ASP		285	-36.143	83.564	15.250		28.76	7
	ATOM	182	CB	ASP		285	-37.299	83.057	15.983		35.32	6
	ATOM	183	CG	ASP		285	-38.129	82.098	15.111		33.29	6
	ATOM	184	OD1	ASP		285	-38.881	82.795	14.013		38.15	6
35	ATOM	185	OD2	ASP		285	-39.660	83.729	14.305		34.70	8
55	ATOM	186	C	ASP		285	-38.741	82.406	12.821		34.43	8
	ATOM	187	0	ASP	В		-36.863	82.339	17.257		36.70	6
	ATOM	188	N	PHE	В		-37.606	82.304	18.237		37.96	8
	ATOM	189	CA	PHE		286	-35.663	81.755	17.235		35.96	7
40	ATOM	190	CB	PHE		286	-35.134	81.053	18.401		37.10	6
	ATOM	191	CG	PHE		286	-33.870	80.262	18.052		37.97	6
	ATOM	192		PHE			-33.079	79.818	19.258	-	36.50	6
	ATOM	193		PHE			-33.704	79.168	20.294		36.75	6
	ATOM	194		PHE			-31.721	80.063	19.343		33.83	6
45	ATOM	195		PHE			-32.987	78.769	21.401		39.55	6
	ATOM	196	CZ	PHE			-30.997	79.662	20.456		38.08	6
	ATOM	197	C	PHE			-31.632	79.013	21.486		34.44	6
	ATOM	198	0	PHE			-34.808	82.023	19.504		36.83	6
	ATOM	199					-35.246	81.845	20.631		35.61	8
50	ATOM	200	N	ALA			-34.005	83.027	19.169		37.33	7
50	ATOM		CA	ALA			-33.599	84.035	20.132		36.34	6
		201	СВ	ALA			-32.644	85.008	19.469		36.40	6
	ATOM	202	С	ALA			-34.831	84.769	20.657		38.76	6
	ATOM	203	0	ALA			-34.882	85.193	21.814	1.00	41.98	8
55	ATOM	204	N	LYS			-35.820	84.912	19.779		38.28	7
55	ATOM	205	CA	LYS			-37.066	85.584	20.112		45.26	6
	ATOM	206	CB	LYS			-37.983	85.690	18.898	1.00	48.35	6
	ATOM	207	CG	LYS			-37.577	86.756	17.916	1.00	51.43	6
	ATOM	208	CD	LYS	В	288	-38.806	87.359	17.226	1.00	60.23	6

5	ATOM	209	CE	LYS	В	288	-39.680	86.308	16.564	1.00 62.83	6
	MOTA	210	NZ	LYS	В	288	-38.897	85.460	15.614	1.00 64.69	
	ATOM	211	С	LYS	В	288	-37.846	84.901	21.191	1.00 43.3	
	ATOM	212	0	LYS	В	288	-38.650	85.532	21.857	1.00 45.6	
	ATOM	213	N	LYS	В	289	-37.618	83.604	21.345	1.00 41.70	
10	ATOM	214	CA	LYS	В	289	-38.313	82.849	22.351	1.00 40.6	
	ATOM	215	CB			289	-38.554	81.418	21.845	1.00 42.2	
	ATOM	216	CG	LYS		289	-39.438	81.368	20.589	1.00 39.5	
	ATOM	217	CD			289	-40.093	80.010	20.422	1.00 43.1	
	ATOM	218	CE			289	-41.025	79.987	19.223	1.00 45.7	
15	ATOM	219	NZ	LYS		289	-42.391	80.476	19.512	1.00 52.49	
	ATOM	220	С	LYS			-37.555	82.871	23.668	1.00 41.5	
	ATOM	221	0	LYS			-38.057	82.366	24.657	1.00 39.7	
	ATOM	222	N	LEU		290	-36.365	83.482	23.661	1.00 40.6	
	ATOM	223	CA	LEU			-35.539	83.599	24.854	1.00 39.3	
20	ATOM	224	СВ	LEU		290	-34.053	83.499	24.491	1.00 36.1	
	ATOM	225	CG	LEU		290	-33.640	82.240	23.767	1.00 34.8	
	ATOM	226		LEU		290	-32.147	82.255	23.523	1.00 29.0	
	ATOM	227		LEU			-34.013	81.040	24.607	1.00 33.4	
	ATOM	228	С	LEU			-35.832	84.915	25.577	1.00 40.0	
25	ATOM	229	Ō	LEU			-35.479	86.006	25.088	1.00 42.0	
	ATOM	230	N			291	-36.462	84.840	26.765	1.00 40.2	
	ATOM	231	CD	PRO			-36.819	83.613	27.494	1.00 39.6	
	ATOM	232	CA	PRO			-36.782	86.069	27.501	1.00 33.0	
	ATOM	233	СВ	PRO			-37.376	85.574	28.811	1.00 35.8	
30	ATOM	234	CG			291	-37.549	84.110	28.695	1.00 34.1	
	ATOM	235	С	PRO			-35.570	87.002	27.714	1.00 40.0	
	ATOM	236	0	PRO			-35.625	88.197	27.403	1.00 41.3	
	ATOM	237	N	MET			-34.474	86.476	28.258	1.00 40.5	
	ATOM	238	CA	MET		292	-33.296	87.286	28.545	1.00 42.8	
35	ATOM	239	СВ			292	-32.149	86.376	28.975	1.00 43.2	
	ATOM	240	CG	MET			-32.553	85.302	29.970	1.00 50.3	
	ATOM	241	SD	MET		292	-31.070	84.609	30.755	1.00 51.1	
	ATOM	242	CE	MET	В	292	-31.797	83.212	31.701	1.00 54.6	
	ATOM	243	С	MET		292	-32.895	88.077	27.315	1.00 41.0	
40	ATOM	244	0	MET	В	292	-32.228	89.098	27.420	1.00 39.6	
	ATOM	245	N	PHE	В	293	-33.322	87.604	26.143	1.00 39.3	
	ATOM	246	CA	PHE	В	293	-33.017	88.271	24.878	1.00 40.9	
	ATOM	247	СВ	PHE	В	293	-33.296	87.329	23.707	1.00 40.9	
	ATOM	248	CG			293	-32.937	87.909	22.365	1.00 42.7	
45	ATOM	249	CD1	PHE	В	293	-31.653	88.354	22.120	1.00 44.4	
	ATOM	250		PHE			-33.872	87.972	21.350	1.00 43.6	
	ATOM	251		PHE			-31.306	88.869	20.872	1.00 39.83	
	ATOM	252		PHE			-33.525	88.486	20.100	1.00 46.2	
	ATOM	253	CZ			293	-32.239	88.926	19.859	1.00 45.18	
50	ATOM	254	С			293	-33.873	89.518	24.744	1.00 45.5	
	ATOM	255	0			293	-33.369	90.626	24.579	1.00 42.0	
	ATOM	256	N	CYS			-35.181	89.305	24.808	1.00 47.0	
	ATOM	257·		CYS			-36.146	90.382	24.689	1.00 50.19	
	ATOM	258	СВ	CYS			-37.553	89.793	24.756	1.00 45.90	
55	MOTA	259	SG	CYS			-37.899	88.607	23.449	1.00 43.50	
	ATOM	260	C	CYS			-35.974	91.474	25.751	1.00 51.38	
	MOTA	261	O	CYS			-36.585	92.536	25.656	1.00 53.83	
	ATOM	262	N	GLU			-35.137	91.200	26.753	1.00 49.72	
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5	ATOM	263	CA	GLU	В	295	-34.8	39	92.159	27.816		52.53	6
	ATOM	264	CB	GLU	В	295	-34.5	53	91.412	29.131		57.40	6
	MOTA	265	CG	GLU	В	295	-35.8	11	90.978	29.874		69.63	6
	ATOM	266	CD	GLU	В	295	-36.6	10	92.144	30.375		78.49	6
	ATOM	267	OE1	GLU	В	295	-36.1	53	92.869	31.29	7 1.00	82.82	8
10	ATOM	268	OE2	GLU	В	295	-37.7	30	92.385	29.860	1.00	85.30	8
	ATOM	269	С	GLU	В	295	-33.6	29	93.009	27.415	5 1.00	48.54	6
	ATOM	270	0	GLU	В	295	-32.9	81	93.627	28.260	1.00	49.82	8
	ATOM	271	N	LEU			-33.3	74	93.030	26.109	1.00	43.79	7
	MOTA	272	CA	LEU			-32.2	68	93.761	25.540	1.00	45.42	6
15	ATOM	273	CB	LEU			-31.3	19	92.769	24.83	3 1.00	41.04	6
	ATOM	274	CG	LEU		296	-30.7	35	91.631	25.66	2 1.00	42.74	6
	ATOM	275		LEU		296	-30.3		90.478	24.76	1.00	40.99	6
	ATOM	276		LEU		296	-29.5		92.119	26.46	3 1.00	39.44	6
	ATOM	277	С	LEU		296	-32.7		94.779	24.52	2 1.00	45.56	6
20	ATOM	278	0	LEU		296	-33.8		94.600	23.92	4 1.00	43.07	8
	ATOM	279	N	PRO		297	-32.0		95.875	24.33	8 1.00	46.99	7
	ATOM	280	CD	PRO		297	-30.7		96.123	25.04	6 1.00	47.12	6
	ATOM	281	CA	PRO		297	-32.3		96.912	23.36		49.61	6
	ATOM	282	СВ	PRO		297	-31.2		97.973	23.49		49.91	6
25	ATOM	283	CG	PRO		297	-30.3		97.477	24.54		51.28	6
	ATOM	284	C	PRO			-32.2		96.273	21.91		49.59	6
	ATOM	285	0	PRO			-31.4		95.340	21.68	5 1.00	51.66	8
	ATOM	286	N			298	-33.0		96.667	20.85		51.02	7
	ATOM	287	CA			298	-32.7		96.150	19.45		52.86	6
30	ATOM	288	СВ	CYS			-33.1		97.165	18.35	6 1.00	54.57	6
	ATOM	289	SG	CYS	•		-34.8		97.085	17.83		67.87	16
	ATOM	290	С	CYS		298	-31.3		96.330	19.12	7 1.00	48.51	6
	MOTA	291	0	CYS		298	-30.5		95.506	18.74	4 1.00	49.58	8
	MOTA	292	N	GLU	В	299	-31.3	L07	97.447	19.23	0 1.00	44.17	7
35	ATOM	293	CA	GLU	В	299	-29.9	989	97.645	18.71	8 1.00	47.57	
	MOTA	294	CB	GLU	В	299	-29.4	102	98.973	19.20	8 1.00	49.92	
	ATOM	295	CG	GLU	В	299	-29.9	944	100.187	18.43			
	ATOM	296	CD	GLU	В	299	-31.0	90	100.887	19.16	4 1.00	63.80	
	ATOM	297	OE1	GLU	В	299	-31.0	673	101.904	18.62	9 1.00	69.03	
40	ATOM	298	OE2	GLU	В	299	-31.	173	100.458	20.31			
•	ATOM	299	С	GLU	В	299	-28.	993	96.533	18.98		46.57	
	ATOM	300	0	GLU	В	299	-28.2	200	96.179	18.11	1 1.00	44.65	
	ATOM	301	N	ASP	В	300	-29.0	045	95.989	20.20		45.17	
	ATOM	302	CA	ASP	В	300	-28.	152	94.908	20.58	4 1.00	43.32	
45	ATOM	303	СВ	ASP	В	300	-27.	985	94.849	22.10	5 1.00	37.38	
	MOTA	304	CG	ASP	В	300	-27.	239	96.016	22.65		36.23	
	MOTA	305	OD1	ASP	B	300	-26.	208	96.421	22.05		35.87	
	MOTA	306	OD2	ASP	В	300	-27.	661	96.543	23.71	6 1.00	40.14	
	ATOM	307	С	ASP	В	300	-28.	721	93.591	20.07	1 1.00	42.81	. 6
50	ATOM	308	0	ASP	В	300	-28.	001	92.775	19.48	9 1.00	46.02	
	MOTA	309	N			301		019	93.399	20.30	6 1.00	38.60	7
	MOTA	310	CA	GLN	В	301	-30.	712	92.197	19.85	8 1.00	40.00	6
	ATOM	311	СВ			301	-32.		92.418	19.83		38.59	
	ATOM	312	CG			301			92.380	21.18		40.26	
55	ATOM	313	CD			301			92.583	21.08		44.15	
	ATOM	314		GLN					93.637	20.58		45.73	
	ATOM	315		GLN					91.602	21.54		46.13	
	ATOM	316	C			301			91.830	18.45		41.64	
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5	ATOM	317	0	GLN E	301		-30.162	90.662	18.100		45.02	8
	MOTA	318	N	ILE E	302		-29.916	92.864	17.674		41.01	7
	ATOM	319	CA	ILE E	302		-29.424	92.692	16.311		40.23	6
	MOTA	320	CB	ILE E	302		-29.584	93.978	15.498		39.52	6
	ATOM	321	CG2	ILE E	3 3 0 2		-29.034	93.792	14.100		31.98	6
10	MCTA	322	CG1	ILE E	3 302		-31.059	94.385	15.416		40.77	6
	MOTA	323	CD1	ILE E	3 302	!	-31.939	93.317	14.775		45.43	6
	MOTA	324	С	ILE E	3 302		-27.966	92.260	16.342		38.58	6
	MOTA	325	0	ILE F	3 302		-27.613	91.197	15.830		40.81	8
	MOTA	326	N	ILE E	3 303	}	-27.128	93.111	16.933		37.50	7
15	ATOM	327	CA	ILE E	3 303	}	-25.692	92.846	17.062		39.33	6
	ATOM	328	CB	ILE I	3 303	3	-25.066	93.648	18.203		39.06	6
	ATOM	329	CG2	ILE !	3 30:	3	-23.566	93.405	18.257		36.19	6
	ATOM	330	CG1	ILE I	3 30:	3	-25.309	95.143	18.020		40.15	6
	ATOM	331	CD1	ILE I	3 30	3	-24.816	95.966	19.173		36.93	6
20	ATOM	332	С	ILE I	3 30	3	-25.470	91,365	17.323		36.49	6
	ATOM	333	0	ILE !	3 30	3	-24.619	90.725	16.712		36.58	8
	ATOM	334	N	LEU I	30	1	-26.244	90.843	18.266	1.00	32.91	7
	ATOM	335	CA	LEU :	B 30	1	-26.194	89.433	18.633	1.00	27.55	6
	MOTA	336	CB	LEU :	B 30	1	-27.172	89.182	19.793	1.00	22.35	6
25	ATOM	337	CG	LEU	в 30	1	-26.623	89.449	21.187		26.88	6
	ATOM	338	CD1	LEU	в 30	1	-25.540	90.495	21.136		24.82	6
	ATOM	339	CD2	LEU	B 30	4	-27.747	89.840	22.121		23.69	6
	ATOM	340	С	LEU	в 30	4	-26.505	88.547	17.425		28.05	6
	ATOM	341	0	LEU		4	-25.668	87.751	16.983		24.68	8
30	ATOM	342	N	LEU	B 30	5	-27.716	88.700	16.897		26.34	7
	MOTA	343	CA	LEU	в 30	5	-28.145	87.939	15.741		30.91	6
	ATOM	344	CB	LEU			-29.460	88.514	15.199		32.50	6
	ATOM	345	CG	LEU		5	-30.699	88.305	16.050		33.36	6
	MOTA	346		LEU			-31.938	88.839	15.342		33.87	6
35	ATOM	347	CD2		, .		-30.863	86.812	16.298		31.72	6
	MOTA	348	С	LEU			-27.072	87.922	14.666		29.76	6
	ATOM	349	0	LEU			-26.687	86.860	14.202		29.33	8
	MOTA	350	Ŋ		<u>в</u> 30		-26.597	89.107	14.291		29.72	7
	MOTA	351	CA		B 30		-25.576	89.254	13.264		34.28	6
40	MOTA	352	CB		B 30		-25.224	90.732	13.077		35.98	6
	ATOM	353	CG	LYS			-26.350	91.581	12.494		43.35	6
	ATOM	354	CD	LYS			-25.852	92.987	12.182		51.50	6
	ATOM	355	CE	LYS			-24.706	92.932	11.190		53.26	6
	ATOM	356	NZ	LYS			-23.883	94.161	11.251		59.61	7
45	ATOM	357	С	LYS			-24.308	88.484	13.556		35.25	6
	ATOM	358	0	LYS			-23.681	87.917	12.653		33.95	8
	MOTA	359	N	GLY			-23.918	88.478	14.829		35.79	7
	ATOM	360	CA	GLY			-22.702	87.793	15.227		34.59	6
	MOTA	361	C	GLY			-22.811	86.291	15.383		33.80	6
50	MOTA	362	0		B 30		-21.944	85.564	14.895		31.59	8
	MOTA	363	N		B 30		-23.861	85.843	16.071		31.15	7
	ATOM	364	CA		B 30		-24.069	84.434	16.320		29.04	6
	MOTA	365	CB		B 30		-24.761	84.240	17.663		27.59	6
_	ATOM	366	SG		B 30		-26.496	84.629	17.608		30.50	16
55	MOTA	367	С		B 30		-24.911	83.712	15.266		30.59	6
	ATOM	368	0		B 30		-25.088	82.499	15.365		33.77	8
	ATOM	369	N		B 30		-25.432	84.429	14.266		28.46	7
	ATOM	370	CA	CYS	B 30	9	-26.270	83.787	13.265	1.00	30.10	6

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5	ATOM	371	СВ	CYS	В	309	-26.706	84.761	12.194		33.43	6
	ATOM	372	SG	CYS	В	309	-27.875	84.011	11.089		35.20	16
	MOTA	373	С	CYS	В	309	-25.617	82.608	12.603	1.00	27.72	6
	ATOM	374	0	CYS	В	309	-26.170	81.518	12.610	1.00	27.69	8
	ATOM	375	N	MET	B	310	-24.447	82.829	12.011	1.00	26.15	7
10	ATOM	376	CA	MET	В	310	-23.737	81.748	11.352	1.00	26.06	6
	ATOM	377	CB	MET	В	310	-22.439	82.263	10.712	1.00	25.32	6
	ATOM	378	CG	MET	В	310	-21.584	81.157	10.080	1.00	24.08	6
	ATOM	379	SD	MET		310	-22.555	80.324	8.758	1.00	27.71	16
	ATOM	380	CE	MET		310	-21.549	78.826	8.427	1.00	28.50	6
15	ATOM	381	С	MET			-23.416	80.673	12.374	1.00	25.94	6
	ATOM	382	Ō	MET		310	-23.659	79.489	12.151		28.09	8
	ATOM	383	N	GLU			-22.865	81.117	13.500	1.00	25.39	7
	ATOM	384	CA	GLU			-22.466	80.231	14.576		27.03	6
	ATOM	385	СВ	GLU			-22.036	81.048	15.797		24.39	6
20	ATOM	386	CG	GLU			-21.019	82.141	15.509		26.00	6
20	ATOM	387	CD	GLU			-20.524	82.835	16.740		23.95	6
	ATOM	388	OE1	GLU			-21.321	83.108	17.668		19.72	8
	ATOM	389	OE2	GLU			-19.313	83.163	16.815		26.51	8
	ATOM	390	C	GLU			-23.582	79.264	14.964		27.51	6
25	ATOM	391	0	GLU		311	-23.347	78.068	15.093		29.67	8
23	ATOM	392	N	ILE		312	-24.794	79.792	15.145		26.82	7
	ATOM	393	CA	ILE			-25.933	78.967	15.527		25.71	6
	ATOM	394	CB	ILE		-	-27.125	79.814	16.021		23.35	6
	ATOM	395	CG2	ILE	-	312	-28.327	78.933	16.276		20.27	6
30	ATOM	396	CG1	ILE		312	-26.771	80.541	17.325		20.88	6
30	ATOM	397	CD1	ILE		312	-27.952	81.163	18.028		18.15	6
	ATOM	398	CDI	ILE		312	-26.370	78.072	14.392		27.91	6
	ATOM	399	0	ILE		312	-26.769	76.926	14.605		28.96	8
	ATOM	400	N			313	-26.303	78.603	13.174		27.66	7
35	ATOM	401	CA	MET		313	-26.696	77.832	11.999		30.18	6
23	ATOM	401	CB	MET		313	-26.696	78.691	10.734		36.89	6
	ATOM	402	CG	MET			-27.882	79.634	10.607		37.95	6
	ATOM	404	SD	MET			-28.238	80.275	8.907		42.38	16
	ATOM	405	CE	MET			-26.787	81.316	8.639		40.68	6
40	ATOM	406	C	MET			-25.791	76.632	11.808		27.43	6
40		407	0			313	-26.258	75.501	11.893		28.61	8
	ATOM	407	_			314	-24.508		11.549		24.88	7
	ATOM		N			314	-23.533	75.824	11.346		27.98	6
	ATOM	409	CA			314	-23.333	76.441	11.165		29.64	6
45	ATOM	410	CB						12.227		43.44	8
43	ATOM	411	OG			314	-21.844	77.316			22.30	6
	ATOM	412	C			314	-23.514	74.774	12.465		24.18	
	ATOM	413	0			314	-23.279	73.592	12.199			8
	MOTA	414	N			315	-23.760	75.187	13.714		23.99	7
~^	ATOM	415	CA			315	-23.792	74.219	14.811		25.07	6
50	ATOM	416	CB			315	-24.095	74.869	16.169		19.11	6
	ATOM	417	CG			315	-24.507	73.860	17.234		20.39	6
	MOTA	418				315	-23.390	72.878	17.493		18.92	6
	ATOM	419	CD2			315	-24.895	74.560	18.514		12.93	6
<i>-</i> -	ATOM	420	С			315	-24.892	73.219	14.517		24.53	6
55	ATOM	421	0			315	-24.672	72.014	14.550		26.32	8
	ATOM	422	N			316	-26.079	73.762	14.254		28.18	7
	MOTA	423	CA			316	-27.278	72.996	13.971		27.54	6
	MOTA	424	CB	ARG	В	316	-28.432	73.941	13.651	1.00	27.39	6

_		405	66	ADC D 31	6	-28.823	74.857	14.809	1.00 2	2.00	6
5	ATOM	425		ARG B 31		-30.074	75.657	14.451	1.00 1		6
	ATOM	426		ARG B 31			75.944	15.598	1.00 2		7
	ATOM	427		ARG B 31		-30.905	76.337	15.489	1.00 3		6
	MOTA	428		ARG B 31		-32.166		14.280	1.00		7
	MOTA	429		ARG B 31		-32.686	76.535	16.581	1.00		7
10	MOTA	430		ARG B 31		-32.900	76.542		1.00 2		6
	ATOM	431		ARG B 31		-27.128	72.028	12.830	1.00		8
	MOTA	432		ARG B 31		-27.852	71.053	12.760	1.00		7
	ATOM	433		ALA B 31		-26.187	72.309	11.941			6
	MOTA	434		ALA B 31		-25.938	71.466	10.794	1.00		6
15	ATOM	435	CB	ALA B 3		-25.337	72.300	9.675	1.00		
	ATOM	436	С	ALA B 3		-24.998	70.327	11.150	1.00		6
	ATOM	437	0	ALA B 3		-25.223	69.187	10.773	1.00		8
	ATOM	438	N	ALA B 3	18	-23.941	70.659	11.882	1.00		7
	ATOM	439	CA	ALA B 3	18	-22.957	69.682	12.299	1.00		6
20	ATOM	440	CB	ALA B 3	18	-21.915	70.355	13.160	1.00		6
	ATOM	441	С	ALA B 3	18	-23.645	68.591	13.084	1.00		6
	ATOM	442	0	ALA B 3	18	-23.415	67.415	12.854	1.00		8
	MOTA	443	N	VAL B 3	19	-24.502	69.012	14.016	1.00		7
	MOTA	444	CA	VAL B 3	19	-25.259	68.107	14.889		35.24	6
25	ATOM	445	СВ	VAL B 3	19	-26.228	68.897	15.765		27.34	6
	ATOM	446	CG1	VAL B 3	19	-25.576	70.149	16.246		29.96	6
	ATOM	447	CG2	VAL B 3	19	-27.505	69.212	15.022		31.70	6
	ATOM	448	С	VAL B 3	19	-26.066	67.146	14.043		40.01	6
	ATOM	449	0	VAL B 3	19	-26.701	66.250	14.578		42.70	8
30	ATOM	450	N	ARG B 3		-26.025	67.353	12.723		38.64	7
50	ATOM	451	CA	ARG B 3		-26.770	66.541	11.762		38.61	6
	ATOM	452	CB		320	-27.838	67.409	11.123		37.26	6
	ATOM	453	CG		320	-29.152	67.280	11.822		43.12	6
	ATOM	454	CD	7	320	-30.145	68.340	11.387		50.79	6
35	ATOM	455	NE	•••,	320	-31.500	67.911	11.705		54.71	7
55	ATOM	456	CZ		320	-32.555	68.723	11.597		57.89	6
	ATOM	457			320	-32.398	69.957	11.130		49.08	7
	ATOM	458		ARG B 3		-33.773	68.302	11.844		59.59	7
	ATOM	459	С	ARG B		-25.937	65.910	10.670		42.14	6
40	ATOM	460	0	ARG B 3		-26.381	65.802	9.532		46.30	8
40	ATOM	461	N	TYR B		-24.734	65.488	11.022		42.04	7
	ATOM	462	CA	TYR B		-23.858	64.848	10.063	1.00	42.70	6
	ATOM	463		TYR B		-22.433	65.332	10.297	1.00	38.01	6
	ATOM	464		TYR B	<i>2</i> .	-21.393		9.756	1.00	37.94	6
45	ATOM	465		TYR B		-21.265		8.397	1.00	33.85	6
43	ATOM	466		TYR B		-20.333		7.912		34.49	6
	MOTA	467		TYR B		-20.583		10.613		28.03	6
		468		-		-19.658		10.134		32.69	6
	ATOM			TYR B		-19.532		8.781		35.18	6
50	ATOM	469		TYR B		-18.616		8.292		39.48	8
50		470				-23.897		10.234		45.51	6
	ATOM	471		TYR B		-23.560		11.292		48.02	8
	ATOM	472		TYR B						44.56	7
	ATOM	473		ASP B		-24.317				45.86	6
	MOTA	474		ASP B		-24.391				46.64	6
55		475		ASP B		-25.570				40.00	6
	ATOM	476		ASP B		-25.449				40.00	8
	MOTA	477		1 ASP B		-24.388				40.00	8
	ATOM	478	OD:	2 ASP B	322	-26.414	58.862	7.117	1.00	40.00	0

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5	ATOM	533		THR	B 329	-29.43	2 69.80	1 7.535	3 1.00 43.72	
	ATOM	534	N	LEU	B -330	-28.58				
	ATOM	535	CA	LEU :	B 330	-28.98				
	ATOM	536	СВ	LEU :	B 330	-28.35				_
	ATOM	537		LEU 1	B 330	-26.84				
10	ATOM	538	CD	1 LEU		-26.22				
	ATOM	539		2 LEU 1		-26.36				
	ATOM	540	С		B 330	-30.508				
	ATOM	541	0		В 330	-31.211				
	ATOM	542	N		331	-30.988		_		
15	ATOM	543	CA		3 331	-32.407				
	ATOM	544	СВ		3 331	-32.870				6
	ATOM	545		ASN E		-33.687				6
	ATOM	546		l ASN E						
	ATOM	547		2 ASN E		-33.182				8
20	ATOM	548		ASN E		-34.935				7
	ATOM	549		ASN E		-33.251			1.00 58.00	6
	ATOM	550		GLY E		-34.464				8
	ATOM	551	CA	GLY E		-32.596			1.00 58.45	7
	ATOM	552	C	GLY E		-33.295			1.00 58.55	6
25	ATOM	553	0	GLY B		-33.909			1.00 59.79	6
	ATOM	554	N	GLU B		-34.609			1.00 61.32	8
	ATOM	555	CA	GLU B		-33.639			1.00 60.28	7
	ATOM	556	CB	GLU B		-34.196			1.00 59.13	6
	ATOM	557	CG	GLU B		-34.966			1.00 62.40	6
30	ATOM	558	CD			-36.099			1.00 75.69	6
	ATOM	559		GLU B	333	-36.720	72.135	2.998	1.00 80.41	6
	ATOM	560	OE2	GLU B	333	-35.984	73.081	2.618	1.00 79.98	8
	ATOM	561	C C			-37.966	72.158	2.830	1.00 83.81	8
	ATOM	562		GLU B	333	-33.110	68.722	2.624	1.00 57.18	6
35	ATOM	563	0	GLU B		-33.236	67.689	1.974	1.00 57.50	8
20	ATOM	564	N		334	-32.054	69.528	2.539	1.00 55.20	7
	ATOM	565	CA	MET B	334	-30.926	69.259	1.653	1.00 50.85	6
	ATOM		CB	MET B	334	-30.514	70.563	0.984	1.00 48.70	6
	ATOM	566	CG	MET B	**	-29.244	70.460	0.194	1.00 45.39	6
40	ATOM	567	SD	MET B		-28.743	72.008	-0.624	1.00 44.56	16
40	ATOM	568	CE			-30.307	72.445	-1.503	1.00 45.25	6
		569	С	MET B		-29.711	68.634	2.319		6
	ATOM	570	0	MET B		-29.185	69.161	3.291	1.00 52.52	8
	ATOM	571	N	ALA B		-29.270	67.515	1.758	1.00 51.00	7
45	ATOM	572	CA	ALA B		-28.106	66.802	2.267	1.00 48.98	6
43	ATOM	573	CB	ALA B		-28.377	65.304	2.274	1.00 47.86	6
	ATOM	574	С	ALA B		-26.931	67.108	1.371	1.00 51.01	6
	ATOM	575	0	ALA B		-26.936	66.760	0.190	1.00 51.61	8
	ATOM	576	N	VAL B		-25.921	67.770	1.930	1.00 46.62	7
50	ATOM	577	CA	VAL B		-24.730	68.142	1.152	1.00 42.35	
50	ATOM	578	CB	VAL B		-24.466	69.635	1.258	1.00 42.33	6
	ATOM	579		VAL B		-25.695	70.418	0.860	1.00 42.41	6
	ATOM	580	CG2	VAL B	336	-24.018	70.004	2.642		6
	ATOM	581		VAL B		-23.493	67.390	1.611	1.00 40.32	6
	ATOM	582		VAL B		-23.464	66.775	2.681	1.00 45.33	6
55	ATOM	583		THR B		-22.461	67.478		1.00 47.42	8
	ATOM	584		THR B		-21.172	66.818	0.781	1.00 41.60	7
	ATOM	585		THR B		-20.720		1.041	1.00 39.69	6
	ATOM	586		THR B		-20.273	66.011	-0.173	1.00 41.35	6
				***		20.273	66,887	-1.213	1.00 49.35	8

		_	01 060	65.175 -	0.702 1	.00 40.38	6
5	ATOM	587 CG2 THR B 337				00 37.88	6
	ATOM	588 C THR B 337		67.846		.00 34.06	8
	MOTA	589 O THR B 337		68.975		1.00 37.61	7
	MOTA	590 N ARG B 338		67.417		1.00 38.68	6
	ATOM	591 CA ARG B 338	_	68.241		1.00 35.95	6
10	ATOM	592 CB ARG B 338		67.333		1.00 33.33	6
	ATOM	593 CG ARG B 338		68.042	-	1.00 35.88	6
	ATOM	594 CD ARG B- 338	-14.348	67.029	• • • • •	1.00 37.42	7
	ATOM	595 NE ARG B 338	-14.520	66.239		1.00 37.42	6
	ATOM	596 CZ ARG B 338	-14.274	66.669		1.00 30.20	7
15	ATOM	597 NH1 ARG B 338	-13.794	67.892	_		7
13	ATOM	598 NH2 ARG B 338	-14.481	65.847	-	1.00 27.40	6
	ATOM	599 C ARG B 338	-17.581	69.075		1.00 38.09	8
	ATOM	600 O ARG B 338	-17.537	70.299	1.284	1.00 34.12	7
	ATOM	601 N GLY B 339	-17.345	68.383	0.117	1.00 41.25	
20		602 CA GLY B 339	-16.981	69.054	-1.119	1.00 41.35	6
20	ATOM	603 C GLY B 339	-18.004	70.109	-1.460	1.00 41.23	6
	MOTA	604 O GLY B 339	-17.736	71.291	-1.330	1.00 38.30	8
	ATOM	605 N GLN B 340	-19.174	69.665	-1.909	1.00 38.58	7
	MOTA	606 CA GLN B 340	-20.258	70.564	-2.276	1.00 40.79	6
	MOTA	• _	-21.596	69.843	-2.079	1.00 40.82	6
25	MOTA		-21.830	68.657	-3.029	1.00 41.10	6
	MOTA		-23.154	67.937	-2.783	1.00 48.84	6
	MOTA		-23.353	67.313	-1.715	1.00 50.53	8
	MOTA		-24.050	68.015	-3.753	1.00 54.25	7
	MOTA		-20.239	71.872	-1.475	1.00 41.50	6
30	MOTA		-20.114	72.958	-2.032	1.00 42.72	8
	MOTA		-20.352	71.736	-0.156	1.00 42.00	7
	MOTA		-20.375	72.879	0.746	1.00 38.10	6
	ATOM	615 CA LEU B 341	-20.401	72.419	2.201	1.00 36.66	6
	MOTA	616 CB LEU B 341	-20.678	73.514	3.194	1.00 39.94	6
35		617 CG LEU B 341	-22.088	74.038	2.936	1.00 34.98	6
	ATOM	618 CD1 LEU B 341	-20.570	72.990	4.609	1.00 40.95	6
	MOTA	619 CD2 LEU B 341	-19.170	73.763	0.543	1.00 36.37	6
	MOTA	620 C LEU B 341	-19.293	74.974	0.497	1.00 37.89	8
	MOTA	621 O LEU B 341	-18.003	_	0.433	1.00 33.29	7
40	MOTA	622 N LYS B 342	-16.737		0.239	1.00 35.17	6
	MOTA	623 CA LYS B 342			0.176	1.00 34.97	6
	ATOM	624 CB LYS B 342	-15.603		0.306	1.00 40.00	6
	ATOM	625 CG LYS B 342	-14.210		0.316	1.00 34.48	6
	MOTA	626 CD LYS B 342	-13.155		0.755	1.00 37.54	6
4.	5 ATOM	627 CE LYS B 342	-11.775			1.00 42.32	7
	ATOM	628 NZ LYS B 342	-10.790			1.00 38.29	6
	MOTA	629 C LYS B 342	-16.744				8
	MOTA	630 O LYS B 342	-16.725				
	MOTA	631 N ASN B 343	-16.760				
5		632 CA ASN B 343	-16.762		-3.481	_	
,	ATOM	242	-16.97				
	ATOM		-16.178	3 72.272			0
	MOTA		-14.93				
	MOTA		-16.87	7 71.144	-4.259		
E			-17.89	4 75.624			
3		301 D 242	-17.83) -4.284		
	ATOM	5 344	-18.93				7
	ATOM					9 1.00 39.25	6
	ATOM	1 640 CA GLY B 344	_				

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5	ATOM	641	С	GLY	В	344	-19.867	77.6	536	-2.258	1.00	38.26	6
	ATOM	642	0	GLY	В	344	-20.715	78.5	501	-2.484	1.00	35.69	8
	ATOM	643	N	GLY	В	345	-18.724	77.8	371	-1.619	1.00	35.89	7
	ATOM	644	CA	GLY	В	345	-18.426	79.2	209	-1.159	1.00	34.00	6
	ATOM	645	С	GLY	В	345	-17.848	79.2	298	0.230	1.00	38.64	6
10	MOTA	646	0	GLY	В	345	-17.216	80.3	303	0.573	1.00	38.14	8
	ATOM	647	N	LEU		346	-18.071	78.2		1.041		39.52	7
	ATOM	648	CA	LEU		346	-17.563	78.2		2.403		36.05	6
	ATOM	649	СВ	LEU		346	-18.311	77.2		3.269		35.72	6
	ATOM	650	CG	LEU		346	-19.800	77.4		3.378		34.89	6
15	ATOM	651	CD1	LEU		346	-20.322	76.6		4.554		44.09	6
	ATOM	652	CD2	LEU		346	-20.086	78.9		3.612		34.84	6
	ATOM	653	C	LEU		346	-16.079	78.0		2.445		33.52	6
	ATOM	654	Ö	LEU		346	-15.392	78.3		3.394	1.00		8
	ATOM	655	N	GLY		347	-15.586	77.3		1.385	1.00		7
20	ATOM	656	CA	GLY		347	-14.174	77.0		1.305	1.00		6
20	ATOM	657	C	GLY		347	-13.768	76.2		2.477	1.00		6
	ATOM	658	0	GLY		347	-14.433	75.2		2.808	1.00		8
	ATOM	659	N	VAL		348	-14.433	76.5		3.087	1.00	31.30	7
	ATOM	660	CA	VAL		348	-12.097	75.8		4.227	1.00		6
25	ATOM	661	CB		В	348	-10.889	76.6		4.227	1.00		
23	ATOM	662	CG1		В	348	-11.292	77.9		5.360		20.19	6
	ATOM	663	CG2		B	348	-10.250	75.		5.905		24.77	6
	ATOM	664	C		B	348	-13.136	75.0		5.360		33.84	6 6
	ATOM	665	0	VAL		348	-13.136	74.		6.153		29.99	8
30	ATOM	666	N	VAL		349	-14.157	76.5		5.449		33.31	7
50	ATOM	667	CA	VAL		349	-15.147	76.3		6.483		32.23	6
	MOTA	668	CB	VAL		349	-16.226	77.		6.476		32.59	6
	ATOM	669	CG1		- /	349	-17.342	76.9		7.399		33.68	6
	ATOM	670	CG2	VAL		349	-15.667	78.		6.959	1.00		6
35	ATOM	671	C	VAL	•	349	-15.792	74.9		6.380	1.00		6
22	ATOM	672	0	VAL	•••	349	-16.055	74.		7.394		33.73	8
	ATOM	673	N	SER	1.3	350	-16.054	74.		5.176	1.00		7
	ATOM	674	CA	SER		350	-16.695	73.2		5.100	1.00		6
	ATOM	675	CB	SER		350	-16.772	72.		3.684		24.95	6
40	ATOM	676	OG	SER		350	-17.538	71.		3.644		23.16	8
•••	ATOM	677	C	SER	٠.	350	-15.910	72.2		5.942		31.59	6
	ATOM	678	0	SER			-16.417	71.8		6.950		37.62	
	ATOM	679	N	ASP			-14.675	71.9		5.565		28.60	8 7
	ATOM	680	CA	ASP	-		-13.905	71.0		6.378		29.82	6
45	ATOM	681	CB	ASP			-12.419	71.		6.050		27.49	6
	ATOM	682	CG	ASP			-12.151	71.0		4.585		30.22	
	ATOM	683		ASP			-12.131					32.61	6
	ATOM	684		ASP				72.		3.954			8
	ATOM	685					-12.064	69.9		4.017		30.02	8
50	MOTA	686	С	ASP			-14.176	71.3		7.861		30.63	6
50	ATOM	687	0	ASP			-14.458	70.4		8.681		29.54	8
			N	ALA			-14.111	72.		8.177		25.33	7
	ATOM	688	CA	ALA			-14.346	73.0		9.533		28.59	6
	ATOM	689	CB	ALA			-14.252	74.0		9.572		20.95	6
55	ATOM	690	С	ALA			-15.690	72.0		10.086		29.69	6
55	ATOM	691	0	ALA			-15.757	72.0		11.164		30.36	8
	MOTA	692	N	ILE			-16.754	72.8		9.330		27.63	7
	ATOM	693	CA	ILE			-18.096	72.		9.729		27.55	6
	ATOM	694	CB	ILE	В	453	-19.144	73.:	129	8.800	1.00	28.04	6

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5	ATOM	695	CG2	ILE B 353	-20.529	72.673	9.195	1.00 23.68	6
	ATOM	696		ILE B 353		74.657	8.869	1.00 27.33	6
	ATOM	697	CD1	ILE B 353	-20.141	75.313	7.964	1.00 26.23	6
	ATOM	698	С	ILE B 353	-18.309	71.002	9.775	1.00 30.88	6
	ATOM	699	0	ILE B 353	-19.021	70.499	10.639	1.00 31.22	8
10	ATOM	700	N	PHE B 35	4 -17.728	70.279	8.822	1.00 29.86	7
	ATOM	701	CA	PHE B 35	4 -17.881	68.831	8.797	1.00 31.08	6
	ATOM	702	СВ	PHE B 35	4 -17.461	68.249	7.439	1.00 28.80	6
	ATOM	703	CG	PHE B 35	4 -18.568	68.233	6.405	1.00 28.80	6
	ATOM	704	CD1	PHE B 35	4 -19.031	69.403	5.833	1.00 30.96	6
15	MOTA	705	CD2	PHE B 35	4 -19.150	67.027	6.034	1.00 29.45	6
	ATOM	706	CE1	PHE B 35	4 -20.066	69.362	4.902	1.00 27.12	6
	ATOM	707	CE2	PHE B 35	4 -20.186	66.978	5.104	1.00 25.19	6
	ATOM	708	cz	PHE B 35	4 -20.644	68.146	4.535	1.00 28.09	6
	ATOM	709	С	PHE B 35		68.223	9.913	1.00 29.17	6
20	ATOM	710	0	PHE B 35		67.429	10.700	1.00 32.62	8
	ATOM	711	N	ASP B 35		68.593	9.972	1.00 23.86	7
	ATOM	712	CA	ASP B 35	5 -14.864	68.090	11.005	1.00 25.34	6
	ATOM	713	СВ	ASP B 35	5 -13.582	68.929	11.045	1.00 21.41	6
	ATOM	714	CG	ASP B 35		68.456	10.086	1.00 32.08	6
25	ATOM	715	OD1		5 -12.899	68.069	8.944	1.00 33.58	8
	ATOM	716	OD2	ASP B 35	5 -11.345	68.477	10.450	1.00 33.20	8
	MOTA	717	С	ASP B 35	5 -15.570	68.153	12.357	1.00 27.86	6
	ATOM	718	0	ASP B 35	5 -15.430	67.257	13.182	1.00 32.42	8
	ATOM	719	N	LEU B 35	6 -16.339	69.223	12.561	1.00 26.84	7
30	ATOM	720	CA	LEU B 35	6 -17.085	69.400	13.803	1.00 28.66	6
	ATOM	721	СВ	LEU B 35	66 -17.832	70.742	13.800	1.00 25.37	6
	ATOM	722	CG	LEU B 35	66 -18.655		15.023	1.00 27.61	6
	ATOM	723	CD1	LEU B 35	66 -17.729		16.191	1.00 25.43	6
	ATOM	724	CD2	LEU B 35			14.808	1.00 27.49	6
35	ATOM	725	С	LEU B 35			13.883	1.00 30.44	6
	MOTA	726	0	LEU B 35			14.804	1.00 31.55	8
	MOTA	727	N	GLY B 35			12.891	1.00 32.69	7
	ATOM	728	CA	GLY B 35			12.846	1.00 29.87	6
	ATOM	729	С	GLY B 3			13.279	1.00 33.12	6
40	MOTA	730	O	GLY B 3			14.207	1.00 29.41	8
	ATOM	731	N	MET B 3			12.593	1.00 33.31	7
	MOTA	732		MET B 3			12.902	1.00 35.87	6
	ATOM	733		MET B 3			12.151	1.00 34.56	6
	ATOM	734		MET B 3			10.657	1.00 46.43	6
45	ATOM	735		MET B 3			9.751	1.00 42.13	16
	MOTA	736		MET B 3			10.228	1.00 44.29	6
	ATOM	737		MET B 3			14.392	1.00 33.26	6
	MOTA	738		MET B 3			15.075	1.00 36.39	8
	MOTA	739		SER B 3			14.875	1.00 33.31	7
50	ATOM	740		SER B 3			16.270	1.00 34.39	6
	ATOM	741		SER B 3			16.541	1.00 30.84	6
	ATOM	742		SER B 3			17.825	1.00 47.14	8
	ATOM	743		SER B 3			17.169	1.00 36.43	6
	ATOM	744		SER B 3			17.922	1.00 35.46	8
55	ATOM	745		ren è 3			17.079	1.00 36.74	7
	ATOM	746		LEU B 3			17.889	1.00 35.44	6
	MOTA	747		LEU B 3			17.405	1.00 34.16	6
	MOTA	748	CG	LEU B 3	60 -20.263	3 68.255	17.575	1.00 34.59	6

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ASP B 367

ASP B 367

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5	ATOM	803	CG	ASP		367	-34.	172	68.3	166	21.0	81	1.00	42.43	6
	ATOM	804	OD1	ASP	В	367	-34.	051	68.3	373	19.8	54	1.00	35.95	8
	ATOM	805	OD2	ASP	В	367	-34.	829	67.3	188	21.5	04	1.00	51.42	8
	ATOM	806	С	ASP	В	367	-31.	496	70.2	238	22.9	59	1.00	33.71	6
	ATOM	807	0	ASP	В	367	-30.	791	71.3	188	22.6	24	1.00	38.30	8
10	ATOM	808	N	THR	В	368	-31.	858	69.9	997	24.2	18	1.00	31.06	7
	ATOM	809	CA	THR	В	368	-31.	453	70.8	822	25.3	44	1.00	26.28	6
	MOTA	810	СВ	THR	В	368	-31.	567	70.0	020	26.6	43	1.00	27.30	6
	ATOM	811	OG1	THR	В	368	-32.	916	69.5	578	26.8	24	1.00	33.42	8
	ATOM	812	CG2	THR	В	368	-31.	143	70.8	855	27.8	24	1.00	25.16	6
15	ATOM	813	С	THR	В	368	-30.	025	71.3	315	25.1	81	1.00	21.13	6
	ATOM	814	0	THR	В	368	-29.	746	72.	508	25.1	50	1.00	23.17	8
	ATOM	815	N	GLU	В	369	-29.	123	70.3	354	25.0	72	1.00	21.32	7
	ATOM	816	CA	GLU	В	369	-27.	711	70.6	634	24.9	32	1.00	28.00	6
	ATOM	817	CB	GLU	В	369	-26.	947	69.3	306	24.8	78	1.00	32.79	6
20	ATOM	818	CG	GLU	В	369	-27.	229	68.4	433	26.1		1.00	36.29	6
	ATOM	819	CD	GLU	В	.369	-26.	689	67.0	051	26.0		1.00	41.03	6
	ATOM	820	OE1	GLU		369	-26.		66.3		25.1		1.00	42.05	8
	ATOM	821	OE2	GLU	В	369	-25.		66.		27.0	48	1.00	42.03	8
	ATOM	822	С	GLU	В	369	-27.		71.		23.7			25.57	6
25	ATOM	823	0	GLU	В	369	-26.		72.		23.8			20.56	8
	ATOM	824	N	VAL	В	370	-27.	922	71.	154	22.5			25.39	7
	MOTA	825	CA	VAL	В	370	-27.		71.9		21.3		1.00	25.99	6
	ATOM	826	CB	VAL	Ŗ	370	-28.	457	71.4	429	20.1	30		26.15	6
	MOTA	827	CG1	VAL	В	370	-28.	255	72.3	358	18.9	53	1.00	27.65	6
30	MOTA	828	CG2	VAL	В	370	-28.	014	70.0	021	19.7	88	1.00	17.70	6
	ATOM	829	С	VAL	В	370	-28.	238	73.	346	21.6	76	1.00	26.49	6
	MOTA	830	0	VAL	В	370	-27.	580	74.3	351	21.4	45	1.00	28.16	8
	MOTA	831	N	ALÁ	В	371	-29.	450	73.3	362	22.2	13	1.00	21.01	7
	ATOM	832	CA	ALA	B	371	-30.	145	74.	589	22.5	73	1.00	19.57	6
35	ATOM	833	CB	ALA	В	371	-31.	414	74.3	246	23.3	35	1.00	18.62	6
	ATOM	834	C	ALA	В	371	-29.	256	75.5	501	23.4	01	1.00	23.48	6
	ATOM	835	0	ALĄ	В	371	-28.	936	76.	613	22.9	89	1.00	32.67	8
	ATOM	836	N	LEU	В	372	-28.	860	75.0	800	24.5	71	1.00	22.89	7
	ATOM	837	CA	LEU	В	372	-27.	.999	75.	758	25.4	72	1.00	23.28	6
40	ATOM	838	CB	LEU	В	372	-27.	606	74.1	860	26.6	58	1.00	27.76	6
	ATOM	839	CG	LEU	₿	372	-28.		74.	524	27.6			21.18	6
	ATOM	840		LEU			-28.	.272	73.	529	28.6	48	1.00	27.64	6
	ATOM	841	CD2	LEU	Ď	372	-29.	.198	75.1	801	28.2	84	1.00	20.90	6
	ATOM	842	С	LEU	В	372	-26.	.769	76.2	268	24.7	22	1.00	21.34	6
45	ATOM	843	0	LEU	В	372	-26.	439	77.4	454	24.7	62	1.00	23.16	8
	ATOM	844	N	LEU	В	373	-26.	111	75.3	349	24.0	23	1.00	24.42	7
	ATOM	845	CA	LEU	В	373	-24.	916	75.6	669	23.2	54	1.00	23.78	6
	MOTA	846	CB	LEU	В	373	-24.	525	74.	446	22.3	96	1.00	22.18	6
	ATOM	847	CG	LEU	В	373	-23.	.098	74.2	283	21.9	42	1.00	31.52	6
50	ATOM	848	CD1	LEU	В	373	-22.	196	74.	576	23.1	00	1.00	31.93	6
	ATOM	849	CD2	LEU	В	373	-22.	873	72.8	889	21.4	57	1.00	30.24	6
	ATOM	850	С	LEU	₽	373	-25.	235	76.9	902	22.4	0.5	1.00	25.69	6
	ATOM	851	0	LEU	В	373	-24.	491	77.8	880	22.4		1.00	30.13	8
	MOTA	852	N			374	-26.		76.8		21.7			26.24	7
55	ATOM	853	CA	GLN	В	374	-26.		77.9		20.8			21.60	6
	ATOM	854	CB	GLN	В	374	-28.		77.5		20.2			24.57	6
	ATOM	855	CG			374	-28.		76.3		19.3			21.02	6
	ATOM	856	CD	GLN	В	374	-29.		76.0		18.6			22.86	6

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5	ATOM	857		GLN B 374		-29.720	75.049	18.009	1.00 24.07	8
	MOTA	858	NE2	GLN B 374		-30.473	76.980	18.901	1.00 25.59	7
	ATOM	859	С	GLN B 374		-26.988	79.249	21.569	1.00 20.66	6
	ATOM	860	0	GLN B 374		-26.733	80.307	20.994	1.00 24.47	8
	ATOM	861	N	ALA B 375		-27.429	79.182	22.825	1.00 16.26	7
10	ATOM	862	CA	ALA B 375		-27.639	80.374	23.631	1.00 17.16	6
	ATOM	863	СВ	ALA B 375		-28.435	80.025	24.865	1.00 19.53	6
	ATOM	864	С	ALA B 375		-26.304	80.966	24.025	1.00 25.13	6
	ATOM	865	0	ALA B 375		-26.074	82.154	23.833	1.00 23.81	8
	ATOM	866	N	VAL B 376		-25.433	80.111	24.568	1.00 24.57	7
15	ATOM	867	CA	VAL B 376		-24.102	80.526	24.986	1.00 25.80	6
	ATOM	868	СВ	VAL B 376		-23.192	79.321	25.234	1.00 26.48	6
	ATOM	869	CG1			-21.806	79.780	25.620	1.00 23.20	6
	ATOM	870	CG2			-23.771	78.433	26.310	1.00 19.08	6
	ATOM	871	C	VAL B 376		-23.510	81.403	23.898	1.00 25.69	6
20	ATOM	872	0	VAL B 376		-22.796	82.364	24.166	1.00 27.87	8
20	ATOM	873	N	LEU B 377		-23.827	81.049	22.659	1.00 23.09	7
	ATOM	874	CA	LEU B 377		-23.340	81.774	21.492	1.00 22.86	6
	ATOM	875	CB	LEU B 377		-23.552	80.920	20.230	1.00 18.50	6
	ATOM	876	CG	LEU B 377		-22.756	79.638	20.146	1.00 22.65	6
25	ATOM	877	CD1			-23.221	78.786	19.000	1.00 16.70	6
23	ATOM	878	CD2	LEU B 377		-21.300	79.995	20.000	1.00 19.58	6
	ATOM	879	C	LEU B 377		-24.073	83.102	21.384	1.00 26.14	6
	ATOM	880	Ö	LEU B 377		-23.464	84.164	21.419	1.00 20.62	8
	ATOM	881	N	LEU B 378		-25.396	83.023	21.265	1.00 28.99	7
30	ATOM	882	CA	LEU B 378		-26.228	84.217	21.147	1.00 28.87	6
50	ATOM	883	CB	LEU B 378		-27.696	83.894	21.450	1.00 26.89	6
	ATOM	884	CG	LEU B 378		-28.648	85.068	21.500	1.00 28.83	6
	ATOM	885		LEU B 378		-28.507	85.854	20.225	1.00 27.97	6
	ATOM	886		LEU B 378		-30.072	84.605	21.692	1.00 27.69	6
35	ATOM	887	C	LEU B 378		-25.738	85.280	22.090	1.00 31.09	6
55	ATOM	888	0	LEU B 378		-25.398	86.379	21.651	1.00 31.77	8
	ATOM	889	N	MET B 379		-25.695	84.931	23.376	1.00 31.44	7
	ATOM	890	CA	MET B 379		-25.291	85.851	24.434	1.00 32.62	6
	ATOM	891	СВ	MET B 37		-25.797	85.335	25.793	1.00 31.45	6
40	ATOM	892	CG	MET B 37		-27.332	85.262	25.883	1.00 38.75	6
•	ATOM	893	SD	MET B 37		-28.020	86.915	25.550	1.00 41.27	16
	ATOM	894	CE	MET B 37		-29.814	86.586	25.513	1.00 35.68	6
	ATOM	895		MET B 37		-23.796		24.538	1.00 33.72	6
	ATOM	896		MET B 37		-23.246	86.190	25.633	1.00 36.29	8
45	ATOM	897		SER B 38		-23.152	86.335	23.399	1.00 34.49	7
,,,	ATOM	898		SER B 38		-21.738	86.659	23.391	1.00 33.97	6
	ATOM	899		SER B 38		-21.132		22.010	1.00 31.24	6
	ATOM	900		SER B 38		-21.224		21.696	1.00 39.42	8
	ATOM	901		SER B 38		-21.635		23.705	1.00 39.69	6
50	ATOM	902		SER B 38		-22.084		22,933	1.00 44.64	8
50	ATOM	903		SER B 38		-21.053		24.857	1.00 41.04	7
	ATOM	904				-20.907				6
	ATOM	905				-20.610				6
	ATOM	906				-19.351				8
5.5		907		SER B 38		-19.815				6
55		908		SER B 38		-19.725				8
	ATOM	909		ASP B 38		-18.977				7
	ATOM	910				-17.886				6
	MOTA	31() CA	מכ מ זמת	-	17.000				

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5	MOTA	911	CB	ASP	В	382	-16.727	89.562	23.028		48.39	6
	ATOM	912	CG	ASP			-17.142	88.232	22.471		53.23	6
	ATOM	913	OD1	ASP	В	382	-18.102	87.621	23.002		56.97	8
	ATOM	914	OD2	ASP	В	382	-16.513	87.753	21.480		58.91	8
	ATOM	915	С	ASP	В	382	-18.191	91.172	21.772	1.00	41.09	6
10	ATOM	916	0	ASP	В	382	-17.366	91.899	21.229	1.00	40.93	8
	MOTA	917	N	ARG	В	383	-19.369	90.908	21.224	1.00	42.63	7
	ATOM	918	CA	ARG			-19.698	91.445	19.934	1.00	43.32	6
	ATOM	919	СВ	ARG		383	-21.131	91.101	19.557	1.00	42.31	6
	ATOM	920	CG	ARG		383	-21.619	89.672	19.811		40.83	6
15	ATOM	921	CD	ARG		383	-21.144	88.627	18.804		38.09	6
	ATOM	922	NE	ARG		383	-21.922	87.415	18.943		37.33	7
	ATOM	923	CZ	ARG		383	-21.584	86.250	18.411		38.35	6
	ATOM	924		ARG		383	-20.465	86.143	17.700		33.70	7
	ATOM	925		ARG		383	-22.369	85.196	18.604		35.46	7
20	ATOM	926	C	ARG		383	-19.591	92.958	20.007		44.96	6
20	MOTA	927	0	ARG		383	-20.050	93.577	20.980		45.60	8
		928	N	PRO		384	-18.975	93.579	19.005		45.33	7
	ATOM						-18.395	92.881	17.854		46.85	6
	MOTA	929	CD	PRO		384		95.035	18.947		47.37	6
25	ATOM	930	CA	PRO		384	-18.808		17.764		46.90	6
25	MOTA	931	CB	PRO		384	-17.868	95.255			46.41	6
	ATOM	932	CG	PRO		384	-17.575	93.934	17.187		48.29	6
	ATOM	933	С	PRO		384	-20.125	95.778	18.762			
	ATOM	934	0	PRO	~ .	384	-21.048	95.277	18.120		48.34	8 7
30	ATOM	935	N			385	-20.185	96.994	19.314		49.88	6
30	ATOM	936	CA	GLY			-21.371	97.838	19.192		50.35	6
	ATOM	937	C	GLY		385	-22.410	97.615	20.265		50.70	
	ATOM	938	0	GLY		385	-23.382	98.363	20.374		53.48	8 7
	MOTA	939	N	LEU		386	-22.205	96.557	21.044		49.04	
2.5	ATOM	940	CA	LEU		386	-23.136	96.211	22.101		50.53	6
35	MOTA	941	CB	LEU		386	-22.640	94.972	22.853		45.17	6
	ATOM	942	CG	LEU		386	-22.744	93.653	22.121		48.26	6
	ATOM	943	CD1	LEU		386	-22.122	92.525	22.938		41.68	6 .
	ATOM	944	CD2			386	-24.215	93.376	21.852		38.40	6
	MOTA	945	С	LEU			-23.322	97.357	23.058		52.13	6
40	ATOM	946	0			386	-22.438	98.182	23.234		53.67	8
	MOTA	947	N			387	-24.499	97.398	23.666		53.42	7
	ATOM	948	CA			387	-24.830	98.441	24.624		56.01	6
	ATOM	949	CB			387	-26.223	98.993	24.339		56.47	6
	MOTA	950	С			387	-24.775	97.853	26.024		55.52	6
45	ATOM	951	0			387	-23.798	98.027	26.753		53.75	8
	ATOM	952	N			388	-25.843	97.145	26.371		56.03	7
	ATOM	953	CA	CYS	В	388	-26.000	96.525	27.673		59.57	6
	ATOM	954	CB	CYS	В	388	-27.469	96.134	27.839	1.00	59.23	6
	ATOM	955	SG	CYS	В	388	-28.620	97.392	27.264	1.00	58.64	16
50	ATOM	956	С	CYS	В	388	-25.105	95.283	27.798	1.00	62.18	6
	ATOM	957	0	CYS	В	388	-25.590	94.164	27.868	1.00	67.88	8
	ATOM	958	N	VAL	. в	389	-23.789	95.510	27.824	1.00	60.78	7
	ATOM	959	CA			389	-22.797	94.434	27.959	1.00	57 .7 0	6
	ATOM	960	СВ			389	-21.355	94.976	27.998		57.09	6
55	ATOM	961				389	-20.361	93.832	28.085		59.03	6
	ATOM	962				389	-21.065	95.845	26.791		53.98	6
	ATOM	963	C			389	-23.078	93.642	29.230		57.77	6
	ATOM	964	0			389	-23.727	92.602	29.203		60.94	8
			-									-

5	ATOM	965	N	ALA	В	390	-22.561	94.159	30.332	1.00	52.68	7
	ATOM	966	CA	ALA	В	390	-22.684	93.570	31.659		48.41	6
	ATOM	967	СВ	ALA	В	390		94.681	32.716		45.19	6
	ATOM	968	С			390	-23.905	92.697	31.877		47.63	6
	ATOM	969	0	ALA			-23.784	91.576	32.369		51.95	
10	ATOM	970	N	ARG		391	-25.075	93.216	31.498			8
	ATOM	971	CA	ARG		391	-26.330	92.481	31.656		47.11	7
	ATOM	972	CB	ARG		391	-27.502				51.64	6
	ATOM	973	CG	ARG		391		93.318	31.122		54.22	6
	ATOM	974	CD	ARG			-28.887	92.713	31.430		64.20	6
15	ATOM	975				391	-30.059	93.582	30.929		73.80	6
13	ATOM		NE	ARG		391	-31.361	93.097	31.378		79.76	7
		976	CZ			391	-31.736	93.015	32.656	=	84.27	6
	ATOM	977		ARG		391	-30.887	93.372	33.625	1.00	85.28	7
	ATOM	978		ARG			-32.957	92.566	32.955	1.00	86.84	7
20	ATOM	979	С	ARG		391	-26.277	91.133	30.940	1.00	48.18	6
20	ATOM	980	0	ARG			-26.724	90.119	31.465	1.00	49.57	8
	ATOM	981	N	ILE			-25.743	91.167	29.718	1.00	45.01	7
	MOTA	982	CA	ILE		392	-25.592	89.999	28.867	1.00	48.77	6
	MOTA	983	CB	ILE	В	392	-25.112	90.424	27.469	1.00	46.45	6
	ATOM	984	CG2	ILE	В	392	-24.805	89.221	26.614		42.35	6
25	MOTA	985	CG1	ILE	В	392	-26.178	91.283	26.768	1.00		6
	ATOM	986	CD1	ILE	В	392	-25.762	91.768	25.386	1.00		6
	ATOM	987	С	ILE	В	392	-24.671	88.935	29.462	1.00		6
	MOTA	988	0	ILE	В	392	-25.086	87.780	29.605	1.00		8
	MOTA	989	N	GLU	В	393	-23.431	89.298	29.790	1.00		7
30	MOTA	990	CA	GLU	В	393	-22.504	88.328	30.378	1.00		6
	ATOM	991	СВ	GLU			-21.314	89.022	31.044	1.00		6
	ATOM	992	CG	GLU			-20.063	89.005	30.209	1.00		6
	ATOM	993	CD	GLU			-18.877	89.415	30.203		67.69	6
	ATOM	994	OE1			393	-17.709	89.264	30.656		66.42	8
35	ATOM	995	OE2	GLU		393	-18.897	89.976	32.052		70.64	8
	ATOM	996	С	GLU		393	-23.251	87.477	31.416		49.31	
	ATOM	997	0	GLU		393	-23.226	86.260	31.303		49.51	6
	ATOM	998	N	LYS		394	-23.898	88.153	32.409	1.00		8 7
	ATOM	999	CA			394	-24.721	87.579				
40	ATOM	1000	СВ	LYS		394	-25.594		33.506	1.00		6
	ATOM	1001	C	LYS			-25.626	88.693	34.161	1.00		6
	ATOM	1002	Ö	LYS			-25.772	86.548	32.851	1.00		6
	ATOM	1003	N	TYR			-26.203	85.430	33.329	1.00		8
	ATOM	1004	CA	TYR				86.948	31.719	1.00		7
45	ATOM	1005	CB	TYR			-27.076	86.078	30.938	1.00		6
	ATOM	1005	CG	TYR			-27.621	86.821	29.716	1.00		6
	ATOM	1000					-28.827	87.688	29.980	1.00		6
	ATOM		CD1				-29.204	88.680	29.080	1.00		6
		1008	CE1	TYR			-30.331	89.469	29.309	1.00 5		6
50	ATOM	1009		TYR			-29.596	87.509	31.113	1.00 5	56.47	6
50	ATOM	1010	CE2				-30.723	88.295	31.346	1.00 6	62.60	6
	ATOM	1011	CZ	TYR			-31.090	89.281	30.446	1.00 6	53.18	6
	ATOM	1012	ОН	TYR			-32.189	90.068	30.671	1.00 6	54.46	8
	ATOM	1013	С	TYR			-26.276	84.867	30.485	1.00 3	37.30	6
<i></i>	ATOM	1014	0	TYR			-26.611	83.737	30.825	1.00 3	34.10	8
55	ATOM	1015	N	GLN			-25.213	85.108	29.718	1.00 3		7
	ATOM	1016	CA	GLN			-24.380	84.018	29.244	1.00 3		6
	ATOM	1017	CB	GLN				84.550	28.464	1.00 3		6
	ATOM	1018	CG	GLN	В	396		83.470	28.103	1.00 2		6
								•	•			•

ATOM 1020 OE1 GLN B 396 -20.547 84.930 27.109 1.00 ATOM 1021 NE2 GLN B 396 -21.112 83.032 25.992 1.00 ATOM 1022 C GLN B 396 -23.908 83.207 30.434 1.00 ATOM 1023 O GLN B 396 -23.876 81.986 30.384 1.00 ATOM 1024 N ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1025 CA ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1028 OD1 ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1029 OD2 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1032 N SER B 398 -24.223 82.422 33.257 1.00 ATOM 1033 CA SER B 398 -25.432 82.962 33.138 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -26.633 82.293 33.622 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.544 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.646 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.555 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.555 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.555 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.555 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00	40.51 43.77 46.50 81.34 81.38.62 81.39.20 81.37.80	8, 58, 75, 55, 38, 58, 76, 68, 68, 76, 66, 66, 66
ATOM 1021 NE2 GLN B 396 -21.112 83.032 25.992 1.00 ATOM 1022 C GLN B 396 -23.908 83.207 30.434 1.00 ATOM 1023 O GLN B 396 -23.908 83.207 30.434 1.00 ATOM 1024 N ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1025 CA ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1028 OD1 ASP B 397 -22.617 84.297 33.355 1.00 ATOM 1029 OD2 ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1030 C ASP B 397 -21.343 86.287 33.355 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1032 N SER B 398 -24.023 81.327 33.778 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -26.911 80.997 32.867 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.92 80.100 29.293 1.00 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1051 CB LEU B 400 -21.470 79.642 29.726 1.00	27.21 7 37.13 6 37.36 8 38.61 7 40.37 6 40.51 6 43.77 6 46.50 8 51.34 8 38.62 6 39.20 8 37.84 6 37.80	7 5 3 7 5 5 5 3 3 5 3 7 5 6 8 6 8 7 6 6 6 6 6 6
ATOM 1022 C GLN B 396 -23.908 83.207 30.434 1.00 ATOM 1023 O GLN B 396 -23.876 81.986 30.384 1.00 ATOM 1024 N ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1025 CA ASP B 397 -23.069 83.250 32.717 1.00 ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1028 OD1 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1029 OD2 ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1030 C ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1032 N SER B 398 -24.023 81.327 33.778 1.00 ATOM 1033 CA SER B 398 -25.432 82.962 33.138 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -26.633 82.293 33.622 1.00 ATOM 1036 C SER B 398 -28.995 82.715 34.114 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.872 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1040 CD PHE B 399 -28.260 28.739 1.00 ATOM 1040 CD PHE B 399 -28.260 28.739 1.00 ATOM 1040 CD PHE B 399 -28.260 28.739 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1040 CD PHE B 399 -28.2668 82.056 29.109 1.00 ATOM 1046 CD PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1046 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CB LEU B 400 -21.470 79.642 29.726 1.00	37.13 37.36 38.61 740.37 640.51 643.77 646.50 851.34 838.62 639.20 837.84 637.80 6	5875533537568687666666
ATOM 1023 O GLN B 396 -23.876 81.986 30.384 1.00 ATOM 1024 N ASP B 397 -23.544 83.903 31.508 1.00 ATOM 1025 CA ASP B 397 -23.669 83.250 32.717 1.00 ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1028 OD1 ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1029 OD2 ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1032 N SER B 398 -24.223 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -25.432 82.962 33.138 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -27.830 83.246 33.501 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1046 CZ PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1046 CZ PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1046 CZ PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1040 CB PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CB LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CB LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1050 CB LEU B 400 -21.470 79.642 29.726 1.00	37.36 8 38.61 7 40.37 6 40.51 6 43.77 6 46.50 8 51.34 8 38.62 6 39.20 8 37.84 7 37.80 6 37.80	8765633587668687666666
10 ATOM 1024 N ASP B 397 -23.544 83.903 31.508 1.000 ATOM 1025 CA ASP B 397 -23.069 83.250 32.717 1.000 ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.000 ATOM 1027 CG ASP B 397 -22.617 84.297 33.754 1.000 ATOM 1028 OD1 ASP B 397 -20.337 84.366 33.054 1.000 ATOM 1029 OD2 ASP B 397 -20.337 84.366 33.054 1.000 ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.000 ATOM 1031 O ASP B 397 -24.023 81.327 33.778 1.000 ATOM 1032 N SER B 398 -25.653 82.962 33.138 1.000 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.000 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.000 ATOM 1035 OG SER B 398 -26.633 82.293 33.622 1.000 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.000 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.000 ATOM 1039 CA PHE B 399 -26.546 80.963 31.587 1.000 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.000 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.000 ATOM 1040 CB PHE B 399 -28.211 80.717 28.906 1.000 ATOM 1040 CD PHE B 399 -29.194 79.938 28.355 1.000 ATOM 1040 CC PHE B 399 -29.194 79.938 28.355 1.000 ATOM 1040 CC PHE B 399 -29.194 79.938 28.355 1.000 ATOM 1040 CC PHE B 399 -29.194 79.938 28.355 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1040 CC PHE B 399 -25.658 78.754 30.976 1.000 ATOM 1050 CA LEU B 4000 -21.470 79.664 29.726 1.000 ATOM 1050 CG LEU B 4000 -21.470 79.664 29.726 1.000 ATOM 1050 CG LEU B 4000 -21.470 79.664 29.9726 1.000 ATOM 1053 CD1 LEU B 4000 -21.470 79.664 29.9726 1.000	38.61 7 40.37 6 40.51 6 43.77 6 46.50 8 51.34 8 38.62 6 39.20 8 37.84 7 37.80 6 34.28 6 34.28 6 34.28 6 35.96 6 35.75 6 39.30 6 39.86 6 36.81 6 41.25	7 6 5 6 8 6 8 7 6 6 6 6 6 6
ATOM 1025 CA ASP B 397	40.37 40.51 43.77 646.50 851.34 838.62 839.20 837.84 837.80 8	5 5 5 3 5 3 7 5 6 8 6 8 7 6 6 6 6 6 6
ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1028 OD1 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1029 OD2 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1030 C ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1031 O ASP B 397 -24.023 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.023 82.422 33.267 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -27.830 83.246 33.501 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.7454 80.047 33.433 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1041 CG PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.927 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -22.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -20.121 80.304 29.917 1.00	40.51 43.77 46.50 80.51.34 80.38.62 80.39.20 80.37.84 80.37.80 80.37	5 6 8 8 5 8 7 6 6 6 6 6 6 6
ATOM 1026 CB ASP B 397 -22.617 84.297 33.754 1.00 ATOM 1027 CG ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1028 OD1 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1030 C ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.023 81.327 33.778 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -26.933 83.246 33.501 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -22.5927 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -22.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1050 CG LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1050 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -20.121 80.304 29.917 1.00	43.77 46.50 81.34 81.38.62 81.39.20 81.37.80 81.37	633637668666666
ATOM 1027 CG ASP B 397 -21.360 85.025 33.352 1.00 ATOM 1028 OD1 ASP B 397 -20.337 84.366 33.054 1.00 ATOM 1029 OD2 ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -25.432 82.962 33.138 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -26.633 82.293 33.622 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1044 CE1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -25.558 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.527 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1051 CB LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -21.470 79.642 29.726 1.00	46.50 51.34 38.62 39.20 37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	3 3 5 3 7 5 6 8 6 8 7 6 6 6 6 6 6
ATOM 1028 OD1 ASP B 397	51.34 38.62 39.20 37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	3 5 3 7 6 6 8 6 8 7 6 6 6 6 6 6
15 ATOM 1029 OD2 ASP B 397 -21.343 86.287 33.350 1.00 ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.023 81.327 33.778 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 20 ATOM 1034 CB SER B 398 -27.830 83.246 33.501 1.00 ATOM 1035 OG SER B 398 -27.830 83.246 33.501 1.00 ATOM 1036 C SER B 398 -28.995 82.715 34.114 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1047 C PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1055 CG LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1055 CG LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1055 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1055 CG LEU B 400 -21.470 79.642 29.726 1.00	38.62 39.20 37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	537563687666666
ATOM 1030 C ASP B 397 -24.223 82.422 33.267 1.00 ATOM 1031 O ASP B 397 -24.023 81.327 33.778 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 ATOM 1034 CB SER B 398 -26.633 82.293 33.622 1.00 ATOM 1035 OG SER B 398 -27.830 83.246 33.501 1.00 ATOM 1036 C SER B 398 -28.995 82.715 34.114 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1041 CG PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	38.62 39.20 37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	537563687666666
ATOM 1031 O ASP B 397 -24.023 81.327 33.778 1.00 ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 20 ATOM 1034 CB SER B 398 -27.830 83.246 33.501 1.00 ATOM 1035 OG SER B 398 -28.995 82.715 34.114 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -27.454 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	39.20 37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	37668687666666
ATOM 1032 N SER B 398 -25.432 82.962 33.138 1.00 ATOM 1033 CA SER B 398 -26.633 82.293 33.622 1.00 ATOM 1034 CB SER B 398 -27.830 83.246 33.501 1.00 ATOM 1035 OG SER B 398 -28.995 82.715 34.114 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -26.911 80.997 32.867 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.7454 80.047 33.433 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1041 CG PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	37.84 37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	7 6 6 8 6 8 7 6 6 6 6 6 6
ATOM 1033 CA SER B 398	37.80 34.28 46.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	668687666666
20 ATOM 1034 CB SER B 398 -27.830 83.246 33.501 1.00 ATOM 1035 OG SER B 398 -28.995 82.715 34.114 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -27.454 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.658 78.754 30.976 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	34.28 34.60 38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	68687666666
ATOM 1035 OG SER B 398 -28.995 82.715 34.114 1.00 ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -27.454 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1040 CB PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	46.60 8 38.41 6 39.98 8 34.82 7 35.96 6 35.75 6 39.30 6 39.86 6 36.81 6 41.25	8 6 8 7 6 6 6 6 6
ATOM 1036 C SER B 398 -26.911 80.997 32.867 1.00 ATOM 1037 O SER B 398 -27.454 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 25 ATOM 1039 CA PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.927 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	38.41 39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	6 8 7 6 6 6 6 6 6
ATOM 1037 O SER B 398 -27.454 80.047 33.433 1.00 ATOM 1038 N PHE B 399 -26.546 80.963 31.587 1.00 ATOM 1039 CA PHE B 399 -26.772 79.768 30.781 1.00 ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1045 CE2 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1046 CZ PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1047 C PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.927 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	39.98 34.82 35.96 35.75 39.30 39.86 36.81 41.25	8 7 6 6 6 6 6
ATOM 1038 N PHE B 399	34.82 35.96 35.75 39.30 39.86 36.81 41.25	7 6 6 6 6 6
25 ATOM 1039 CA PHE B 399	35.96 35.75 39.30 39.86 36.81 41.25	6 6 6 6 6
ATOM 1040 CB PHE B 399 -26.892 80.100 29.293 1.00 ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	35.75 (39.30 (39.86 (36.81 (39.41.25 (41.25	6 6 6 6
ATOM 1041 CG PHE B 399 -28.211 80.717 28.906 1.00 ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 ATOM 1044 CE1 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -25.927 77.589 31.256 1.00 ATOM 1050 CA LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1051 CB LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1052 CG LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	39.30 (39.86 (36.81 (41.25 (6 6 6
ATOM 1042 CD1 PHE B 399 -28.466 82.056 29.109 1.00 ATOM 1043 CD2 PHE B 399 -29.194 79.938 28.355 1.00 30 ATOM 1044 CE1 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	39.86 (36.81 (341.25 (6 6 6
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30 ATOM 1044 CE1 PHE B 399 -29.700 82.602 28.739 1.00 ATOM 1045 CE2 PHE B 399 -30.424 80.483 27.987 1.00 ATOM 1046 CZ PHE B 399 -30.677 81.813 28.181 1.00 ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.927 77.589 31.256 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00	41.25	6
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ATOM 1047 C PHE B 399 -25.658 78.754 30.976 1.00 ATOM 1048 O PHE B 399 -25.927 77.589 31.256 1.00 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00		6
ATOM 1048 O PHE B 399 -25.927 77.589 31.256 1.00 35 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.00 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00		6
35 ATOM 1049 N LEU B 400 -24.408 79.187 30.796 1.06 ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.06 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.06 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.06 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.06		6
ATOM 1050 CA LEU B 400 -23.275 78.291 30.945 1.00 ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00		8
ATOM 1051 CB LEU B 400 -21.976 79.091 31.030 1.00 ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00		7
ATOM 1052 CG LEU B 400 -21.470 79.642 29.726 1.00 ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.00		6
ATOM 1053 CD1 LEU B 400 -20.121 80.304 29.917 1.0	0 34.24	6
	0 35.10	6
	0 26.60	6
40 ATOM 1054 CD2 LEU B 400 -21.326 78.488 28.759 1.0	0 29.44	6
	0 38.84	6
ATOM 1056 O LEU B 400 -23.366 76.157 32.007 1.0	0 40.38	8
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ATOM 1072 CB PHE B 403 -24.847 74.715 29.607 1.0		6

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5	ATOM	1073	CG 1	РНЕ В	41	03	-24.557	73.908	28.359	1.00 2	26.97	6
3	ATOM	1073		PHE B			-23.916	74.494	27.272	1.00 2	25.55	6
	ATOM	1075		PHE B			-24.939	72.583	28.271	1.00	19.75	6
	ATOM	1075		PHE B			-23.670	73.765	26.104	1.00 2	27.90	6
	ATOM	1077		PHE B		03	-24.693	71.848	27.102	1.00	22.56	6
10	ATOM	1077		PHE B		03	-24.057	72.439	26.020	1.00	22.24	6
10	ATOM	1079		PHE B			-24.810	72.902	31.329	1.00	28.82	6
		1049		PHE B			-25.092	71.726	31.205	1.00	26.00	8
	ATOM ATOM	1081		GLU B			-23.776	73.335	32.037	1.00	30.25	7
		1081		GLU B			-22.865	72.419	32.712	1.00	34.03	6
15	ATOM ATOM	1082		GLU E			-21.835	73.215	33.527	1.00	39.45	6
13		1083		GLU E			-20.654	72.384	34.068	1.00	47.68	6
	ATOM	1385		GLU E			-19.750	73.129	34.996		54.02	6
	ATOM	1086		GLU E			-19.372	74.290	34.701		57.27	8
	ATOM	1087		GLU E		04	-19.369	72.555	36.048		63.85	8
20	ATOM	1087	C	GLU E		104	-23.645	71.509	33.642		36.01	6
20	ATOM	1088	0	GLU E			-23.470	70.292	33.640		38.64	8
	ATOM	1009	N			105	-24.492	72.131	34.458	•	29.56	7
	MOTA	1090	ca			105	-25.306	71.387	35.405		31.69	6
	MOTA	1091	CB			105	-26.245	72.324	36.173		33.75	6
25	ATOM	1092	CG	HIS I			-25.536	73.185	37.163		34.75	6
23	MOTA	1093		HIS I			-24.234	73.286	37.524		34.58	6
	MOTA MOTA	1094		HIS			-26.223	74.101	37.969		32.43	7
	ATOM	1095		HIS			-25.334	74.703	38.769	1.00	36.15	6
	ATOM	1090		HIS		405	-24.139	74.222	38.511	1.00	39.84	7
30	MOTA	1098	C	HIS			-26.106	70.342	34.648	1.00	34.21	6
30	ATOM	1099	0	HIS		-	-26.087	69.160	35.006	1.00	37.06	8
	ATOM	1100	N	TYR			-26.806	70.776	33.598	1.00	30.83	7
	ATOM	1101	CA	TYR		406	-27.592	69.853	32.796	1.00	28.85	6
	ATOM	1102	CB	TYR			-28.192	70.537	31.579	1.00	31.48	6
35	MOTA	1102	CG	TYR			-28.991	69.576	30.730	1.00	23.49	6
33	MOTA	1104	CD1			406	-30.179	69.047	31.196	1.00	19.42	6
	MOTA	1105	CE1			406	-30.893	68.128	30.441	1.00	23.80	6
	MOTA	1106		TYR		406	-28.525	69.152	29.496	1.00	21.81	6
	ATOM	1107		TYR		406	-29.241	68.228	28.740		24.64	6
40	ATOM	1108	CZ	TYR		406	-30.420	67.713	29.217	1.00	21.56	6
40	ATOM	1109	ОН	TYR			-31.120	66.802	28.480		24.96	8
	ATOM	1110	C	TYR			-26.697	68.725	32.304	1.00	24.24	6
	ATOM	1111	O	TYR			-27.155	67.609	32.110	1.00	27.08	8
	ATOM	1112		ILE			-25.422	69.056	32.084	1.00	25.76	7
45	ATOM	1113		ILE			-24.428	68.092	31.628		33.75	6
,-	ATOM	1114		ILE			-23.090	68.778	31.274	1.00	34.23	6
	MOTA	1115		ILE			-21.959	67.774	31.230	1.00	32.46	6
	ATOM	1116		ILE			-23.214	69.514	29.936	1.00	43.30	6
	ATOM	1117		ILE			-23.655	68.612	28.804	1.00	40.40	6
50	ATOM	1118				407	-24.191		32.658	1.00	39.03	6
50	ATOM	1119				407	-24.178		32.343	1.00	35.18	8
	ATOM	1120		ASN			-23.990			1.00	37.25	7
	ATOM	1121		ASN			-23.739			1.00	37.01	6
	ATOM	1122				408	-23.524				32.27	6
55	ATOM	1123				408	-22.296				33.56	6
,,,	ATOM	1124		l ASN			-21.194				31.99	8
	ATOM	1125		2 ASN			-22.478				31.23	7
	ATOM	1126				408	-24.876				38.14	6
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5	ATOM	1127	0	ASN	В	408	-24.624	64.253	35.105	1.00	42.16	8
	MOTA	1128	N	TYR	В	409	-26.122	65.924	35.003	1.00	35.62	7
	ATOM	1129	CA	TYR	В	409	-27.273	65.024	35.073	1.00	35.91	6
	ATOM	1130	CB	TYR	В	409	-28.597	65.787	34.931	1.00	34.41	6
	MOTA	1131	CG	TYR	В	409	-29.788	64.868	34.685	1.00	38.73	6
10	ATOM	1132	CD1	TYR	В	409	-30.064	63.819	35.549		41.34	6
	ATOM	1133	CE1	TYR			-31.130	62.962	35.309		47.16	6
	ATOM	1134	CD2	TYR			-30.613	65.037	33.579		46.20	6
	ATOM	1135	CE2	TYR		409	-31.684	64.176	33.341		50.74	6
	ATOM	1136	CZ	TYR		409	-31.942	63.143	34.206		50.88	6
15	ATOM	1137	OH	TYR		409	-33.002	62.312	33.978		53.14	8
	ATOM	1138	C	TYR			-27.215	64.020	33.951		38.16	6
	ATOM	1139	0			409	-27.558	62.857	34.111		41.83	8
	ATOM	1140	N			410	-26.824	64.528	32.796		42.25	7
	ATOM	1141	CA			410	-26.734	63.739	31.594		42.83	6
20	ATOM	1142	CB			410	-26.350	64.646	30.441		36.83	6
	ATOM	1143	CG			410	-27.440	65.585	29.945		34.32	6
	ATOM	1144	CD			410	-28.284	64.863	28.917		36.62	6
	ATOM	1145	NE			410	-27.455	64.378	27.829		38.64	7
	ATOM	1146	CZ			410	-27.926	63.656	26.824		35.73	6
25	ATOM	1147	NH1			410	-29.234	63.379	26.782		33.17	7
20	ATOM	1148	NH2	ARG			-27.095	63.227	25.868		32.70	7
	ATOM	1149	C	ARG		410	-25.688	62.664	31.733		46.67	6
	ATOM	1150	0	ARG			-25.859	61.547	31.733	-	41.78	8
	ATOM	1151	N			411	-24.602	63.028	32.413		52.99	7
30	ATOM	1151	CA	LYS			-24.602	62.145	32.413		58.32	6
50	ATOM	1153	CB	LYS		411	-23.471	61.249	33.833		64.99	6
	ATOM	1154	CG	LYS		411	-24.998	60.544	33.968		70.48	6
	ATOM	1155	CD	LYS		411	-24.990	59.887	35.349		77.18	6
	ATOM	1156	CE			411	-26.272	58.944	35.474		84.30	6
35	ATOM	1157	NZ			411	-26.272	58.242	36.809		86.48	7
33	ATOM	1158	C			411	-23.172	61.341	31.365		56.66	6
	ATOM	1159	0			411	-23.172	60.199	31.210		55.47	8
	ATOM	1160	N			412	-23.374	62.026	30.479		54.67	7
	ATOM	1161	CA		•	412	-22.436	61.474	29.214		48.67	6
40	ATOM	1161	CB			412						6
40	ATOM	1163	CG			412	-21.500 -22.559	62.599	28.310 27.784		43.14 41.36	6
	ATOM	1163		HIS				63.501			35.44	
				HIS				64.603	28.299			6
	ATOM	1165					-23.163	63.290	26.539		38.19	7
45	ATOM	1166		HIS			-24.076	64.238	26.353		34.75	6
43	ATOM	1167		HIS			-24.090	65.034	27.396		35.52	7
	ATOM	1168	С			412	-20.894	60.596	29.644		46.35	6
	ATOM	1169	0			412	-20.218	60.892	30.644		42.73	8
	ATOM	1170	N			413	-20.708	59.469	28.973		48.92	7
	ATOM	1171	CA			413	-19.593	58.614	29.371		53.15	6
50	ATOM	1172	CB			413	-20.022	57.147	29.421		55.27	6
	ATOM	1173	CG			413	-20.814	56.823	30.636		58.77	6
	ATOM	1174				413	-22.019	56.223	30.822		61.65	6
	ATOM	1175				413	-20.360	57.159	31.921		60.31	7
	ATOM	1176				413	-21.267	56.758	32.809		63.01	6
55	ATOM	1177				413	-22.270	56.193	32.171		62.93	7
	MOTA	1178	С			413	-18.426	58.862	28.438		53.19	6
	ATOM	1179	0			413	-17.975	57.996	27.699		54.93	8
	MOTA	1180	Ŋ	VAL	В	414	-17.970	60.113	28.521	1.00	53.77	7

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5	ATOM	1181	CA V	AL B	414	-16.845	-	- ·	1.00 51.06	6
-	ATOM		CB V	AL B	414	-17.317	61.498	26.586	1.00 51.49	6
	ATOM			AL B	414	-16.133	62.122	25.891	1.00 45.22	6
	ATOM	1184	CG2 V	AL B	414	-18.095	60.631	25.617	1.00 52.67	6
	ATOM	1185		AL B		-16.096	61.557	28.775	1.00 54.28	6
10	MOTA	1186		AL B		-16.700	62.283	29.574	1.00 55.49	8
10	ATOM	1187		HR B		-14.770	61.466	28.742	1.00 56.28	7
	ATOM	1188		HR B		-13.919	62.234	29.669	1.00 57.83	6
	ATOM	1189		HR B		-12.488	61.686	29.658	1.00 59.64	6
	ATOM	1190		HR B		-11.618	62.572	30.373	1.00 66.69	8
15	ATOM	1191		HR B		-11.988	61.483	28.227	1.00 59.42	6
13	ATOM	1192		HR B		-13.840	63.726	29.352	1.00 56.98	6
	ATOM	1193		HR B		-13.987	64.135	28.216	1.00 55.70	8
	ATOM	1194		IIS B		-13.598	64.522	30.387	1.00 57.44	7
	ATOM	1195		IIS B		-13.485	65.972	30.237	1.00 57.34	6
20	MOTA	1196		is B		-12.114	66.326	29.653	1.00 61.35	6
20	ATOM	1197		is B		-10.968	65.931	30.513	1.00 69.78	6
	ATOM	1198		HIS B		-9.930	65.082	30.307	1.00 71.42	6
	ATOM	1199	ND1 H			-10.756	66.480	31.787	1.00 72.49	7
	ATOM	1200		HIS B		-9.631	65.973	32.281	1.00 75.50	6
25	ATOM	1201		HIS B		-9.120	65.131	31.408	1.00 73.91	7
23	MOTA	1202		HIS B		-14.560	66.515	29.320	1.00 53.79	
	ATOM	1203		HIS B		-14.334	67.477	28.591	1.00 52.81	
	ATOM	1204		PHE E		-15.746	65.921	29.372	1.00 48.05	
	ATOM	1205		PHE E		-16.841	66.329	28.505	1.00 47.99	
30	ATOM	1206			3 417	-18.152	65.694	28.937	1.00 46.11	
50	ATOM	1207			3 417	-19.233	65.781	27.898	1.00 44.27	
	ATOM	1208			3 417	-19.280	64.856	26.870	1.00 41.79	
	MOTA	1209	CD2	PHE E	3 417	-20.118	66.846	27.893	1.00 40.23	
	MOTA	1210	CE1	PHE I	в 417	-20.233	64.959	25.869	1.00 44.30	
35	MOTA	1211	CE2	PHE I	B 417	-21.072	66.955	26.893	1.00 36.80	
	ATOM	1212	CZ	PHE I	B 417	-21.119		25.866	1.00 40.69	
	ATOM	1213	С	PHE I	B 417	-17.020	67.833	28.423	1.00 46.69	
	ATOM	1214	0	PHE !	B 417	-16.799		27.380	1.00 43.35	
	ATOM	1215	N	TRP	B 418	-17.448		29.516	1.00 45.14	
40	ATOM	1216	CA	TRP	B 418	-17.681		29.508	1.00 44.89	
	MOTA	1217	СВ	TRP	B 418	-18.045		30.898	1.00 42.24	
	MOTA	1218	CG	TRP	B 418	-18.162		31.018		
	ATOM	1219	CD2	TRP	B 418	-19.298				
	ATOM	1220	CE2	TRP	B 418	-18.953		_	_	
45	ATOM	1221	CE3	TRP	B 418	-20.560				
	ATOM	1222	CD1	TRP	B 418	-17.223			_	
	MOTA	1223	NE1	TRP	B 418	-17.690				
	MOTA	1224	CZ2	TRP	B 418	-19.819				
	ATOM	1225	cz3	TRP	B 418	-21.422				
50					B 418	-21.069				
	ATOM			TRP	B 418	-16.502				
	ATOM			TRP	B 418	-16.67		_		
	ATOM			PRO	B 419	-15.292			_	
	ATOM				в 419	-14.96				
55					в 419	-14.12			_	
	ATOM			PRO	B 419	-12.95				
	ATOM			PRO	B 419	-13.52			_	
	ATOM				B 419	-14.03	5 71.067	7 27.479	9 1.00 36.2	8 6
		_								

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5	ATOM	1235	0	PRO 1	В	119	-13.690	72.001	26.754		37.08	8
	ATOM	1236	N	LYS 1	В	120	-14.330	69.871	26.976	1.00	35.96	7
	ATOM	1237	CA	LYS	В	420	-14.278	69.609	25.538	1.00	40.82	6
	ATOM	1238	СВ	LYS	В	420	-14.452	68.103	25.271	1.00	40.78	6
	MOTA	1239	CG	LYS	В	420	-13.349	67.214	25.830	1.00	48.62	6
10	ATOM	1240	CD	LYS	в	420	-13.565	65.746	25.480	1.00	55.12	6
_	ATOM	1241	CE	LYS	В	420	-12.427	64.892	26.017	1.00	53.26	6
	ATOM	1242	NZ	LYS			-12.582	63.457	25.608	1.00	52.69	7
	ATOM	1243	С	LYS			-15.414	70.374	24.875	1.00	40.29	6
	ATOM	1244	0	LYS			-15.225	71.015	23.851	1.00	39.66	8
15	ATOM	1245	N	LEU			-16.591	70.300	25.499	1.00	38.33	7
	ATOM	1246	CA	LEU			-17.796	70.958	25.001	1.00	37.60	6
	ATOM	1247	СВ	LEU			-18.970	70.702	25.965	1.00	43.66	6
	ATOM	1248	CG	LEU			-20.370	70.850	25.418	1.00	46.50	6
	ATOM	1249	CD1	LEU			-20.529	69.890	24.255	1.00	45.15	6
20	ATOM	1250	CD2	LEU			-21.383	70.538	26.486	1.00	51.31	6
20	ATOM	1251	C	LEU			-17.547	72.452	24.823		39.59	6
	ATOM	1252	Ö	LEU			-17.975	73.035	23.836	1.00	40.66	8
	ATOM	1253	N	LEU			-16.847	73.059	25.780		39.57	7
	ATOM	1254	CA	LEU			-16.534	74.478	25.715		38.63	6
25	ATOM	1255	CB	LEU			-15.829	74.936	26.992		41.79	6
	ATOM	1256	CG	LEU			-16.714	75.149	28.191	1.00	42.74	6
	ATOM	1257		LEU			-15.911	75.685	29.360		42.89	6
	ATOM	1258	CD2	LEU			-17.783	76.162	27.813		39.27	6
	ATOM	1259	C	LEU			-15.677	74.788	24.513		40.47	6
30	ATOM	1260	Ö	LEU			-15.823	75.846	23.917		47.83	8
50	ATOM	1261	N	MET			-14.789	73.853	24.168		34.27	7
	ATOM	1262	CA	MET			-13.907	74.019	23.024		35.25	6
	ATOM	1263	CB	MET			-12.920	72.858	22.922	1.00	32.56	6
	ATOM	1264	CG	MET			-12.013	72.703	24.125		40.70	6
35	ATOM	1265	SD	MET			-10.345	72.007	23.784		47.65	16
20	ATOM	1266	CE	MET			-10.770	70.538	22.761		47.16	6
	ATOM	1267	c	MET			-14.709	74.100	21.738		35.13	6
	ATOM	1268	0	MET		• •	-14.341	74.807	20.803		29.85	8
	ATOM	1269	N			424	-15.811	73.361	21.704		31.56	7
40	ATOM	1270	CA			424	-16.676	73.354	20.544		32.29	6
-10	ATOM	1271	CB			424	-17.783	72.316	20.736		30.56	6
	ATOM	1272	CG			424	-17.257	70.879	20.843		30.07	6
	ATOM	1273	CD			424	-16.444	70.510	19.611		33.22	6
	ATOM	1274	CE			424	-15.795	69.136	19.706		28.75	6
45	ATOM	1275	NZ			424	-14.655	69.067	20.678		31.01	7
	ATOM	1276	C			424	-17.248	74.754	20.304		29.26	6
	ATOM	1277	Ö			424	-17.439	75.149	19.166		30.22	8
	ATOM	1278	N			425	-17.495	75.499	21.385		23.53	7
	ATOM	1279	CA			425	-18.014	76.852	21.278		28.91	6
50	ATOM	1280	CB			425	-18.278	77.458	22.663		29.44	6
50	ATOM	1281		. VAL			-18.633	78.915	22.547		28.81	6
		1282		VAL			-19.401	76.733	23.354		31.22	6
	ATOM ATOM	1282				425	-19.401	77.682	20.498		32.03	6
		1283	0			425	-17.368	78.465	19.629		31.95	8
55	ATOM ATOM	1284				425	-17.366	77.508	20.827		33.61	7
در		1285				426	-13.721	78.221	20.137		30.76	6
	MOTA	1286				426	-14.645	77.912	20.761		32.34	6
	ATOM	1287				426	-13.270	78.697	21.941		33.07	8
	ATOM	1208	OG1	LIME	. ¤	420	-13.073	10.031	C1.241	1.00	55.0,	Ŭ

5	ATOM	1289	CG2 T	THR B	426	-12.153	78.174	19.782	1.00 25.40	6
3	ATOM	1290		THR B		-14.677	77.742	18.706	1.00 32.53	6
	ATOM	1291		THR B		-14.639	78.530	17.763	1.00 35.19	8
	ATOM	1292		ASP B		-14.749	76.425	18.566	1.00 28.83	7
	ATOM	1293		ASP B		-14.796	75.807	17.257	1.00 35.12	6
10	ATOM	1294		ASP B		-15.096	74.302	17.380	1.00 39.14	6
10	ATOM	1295		ASP B		-13.910	73.496	17.806	1.00 45.80	6
	ATOM	1296		ASP B		-12.786	73.774	17.348	1.00 41.97	8
	ATOM	1297		ASP B		-14.064	72.517	18.583	1.00 50.06	8
	ATOM	1298		ASP B		-15.883	76.502	16.429	1.00 33.94	6
15	ATOM	1299		ASP B		-15.673	76.815	15.262	1.00 38.02	8
13	ATOM	1300		LEU B		-17.040	76.741	17.048	1.00 27.15	7
	ATOM	1301		LEU B		-18.154	77.388	16.367	1.00 29.99	6
	ATOM	1302		LEU B		-19.448	77.190	17.168	1.00 22.49	6
	ATOM	1303		LEU B		-20.086	75.818	17.089	1.00 25.54	6
20	MOTA	1303		LEU B		-21.282	75.729	18.012	1.00 20.60	6
20		1305		LEU B		-20.509	75.564	15.651	1.00 17.24	6
	MOTA	1305		LEU B		-17.901	78.863	16.103	1.00 28.94	6
	MOTA MOTA	1300		LEU B		-18.328	79.388	15.076	1.00 31.26	8
		1307	N	ARG E	•	-17.213	79.524	17.035	1.00 27.64	7
25	MOTA MOTA	1309	CA	ARG E		-16.894	80.937	16.883	1.00 28.13	6
23	ATOM	1310	CB	ARG E		-16.274	81.507	18.160	1.00 29.59	6
	MOTA	1311	CG	ARG E		-17.246	81.752	19.302	1.00 34.85	6
	ATOM	1312	CD	ARG E		-16.626	82.653	20.372	1.00 47.18	6
	ATOM	1313	NE	ARG E		-17.373	82.714	21.620	1.00 57.93	7
30	ATOM	1314	cz	ARG E		-18.632	83.124	21.716	1.00 63.62	6
50	ATOM	1315		ARG I		-19.263	83.579	20.622	1.00 60.71	7
	ATOM	1316		ARG I		-19.238	83.130	22.916	1.00 62.38	7
	MOTA	1317	С	ARG I		-15.930	81.146	15.728	1.00 29.81	6
	ATOM	1318	Ō	ARG I		-16.101	82.061	14.933	1.00 30.81	8
35	MOTA	1319	N		в 430	-14.908	80.295	15.670	1.00 29.64	7
22	ATOM	1320	CA		в 430	-13.920	80.343	14.614	1.00 34.72	6
	MOTA	1321	СВ		в 430	-12.939	79.192	14.763	1.00 34.97	6
	ATOM	1322	CG	MET	B 430	-11.787	79.431	15.689	1.00 45.34	6
	ATOM	1323	SD	MET	B-430	-10.729	80.768	15.158	1.00 52.55	16
40	ATOM	1324	CE	MET	B 430	-10.070	80.157	13.610	1.00 55.56	6
	MOTA	1325	С	MET	B 430	-14.638	80.217	13.284	1.00 34.01	6
	ATOM	1326		MET	B 430	-14.395	80.996		1.00 37.29	8
	MOTA	1327	N	ILE	B 431	-15.516	79.217			7
	ATOM	1328	CA	ILE	B 431	-16.296	78.992			6
45	ATOM	1329	CB	ILE	B 431	-17.391	77.929			6
	ATOM	1330	CG2	ILE	B 431	-18.314	77.841			6
	ATOM	1331	CG1	ILE	B 431	-16.784	76.555		_	6
	MOTA	1332	CD1	ILE	B 431	-17.826	75.464			6
	ATOM	1333	С	ILE	B 431	-16.953	80.288			6
50	ATOM	1334	0	ILE	B 431	-16.837	80.725			8
	ATOM	1335	N	GLY	B 432	-17.657	7 80.904			7
	ATOM	1336	CA	GLY	B 432	-18.357	7 82.142			6
	ATOM	1337		GLY	B 432	-17.395	83.209			6
	ATOM	1338			в 432	-17.531	83.740			8
55					B 433	-16.43				7
	ATOM				B 433	-15.40	7 84.514			6
	ATOM				B 433	-14.240	84.338			6
	ATOM				B 433	-14.90	5 84.433	10.867	1.00 30.73	6

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5	ATOM	1343	0	ALA	В	433	-14.849	85.432	10.171	1.00	31.60	8
	MOTA	1344	N	CYS			-14.534		10.439		33.22	7
	ATOM	1345	CA	CYS			-14.023		9.120		34.34	6
	ATOM	1346	СВ	CYS			-13.553		9.226		35.20	6
	ATOM	1347	SG	CYS			-12.412		8.444		54.48	16
10	ATOM	1348	С	CYS			-15.106		8.062		34.09	6
	ATOM	1349	0	CYS			-14.844		6.952		34.89	8
	ATOM	1350	N	HIS			-16.318		8.394		34.30	7
	ATOM	1351	CA	HIS			-17.395		7.443		35.44	6
	ATOM	1352	СВ	HIS			-18.700		8.103		31.76	6
15	ATOM	1353	CG			435	-19.845		7.149		32.03	6
	ATOM	1354		HIS			-20.483		6.515		28.61	6
	ATOM	1355		HIS			-20.345		6.607		28.48	7
	ATOM	1356		HIS			-21.24		5.672		33.27	6
	ATOM	1357		HIS		435	-21.34		5.605		31.57	7
20	ATOM	1358	С			435	-17.528		6.878		32.74	6
	ATOM	1359	o			435	-17.842		5.715		32.87	8
	ATOM	1360	N			436	-17.31		7.758		31.01	7
	ATOM	1361	CA	ALA		436	-17.37		7.405		29.91	6
	ATOM	1362	CB			436	-17.008		8.618		21.23	6
25	ATOM	1363	C			436	-16.39		6.266		33.86	6
	ATOM	1364	Ö			436	-16.73		5.257		36.10	8
	ATOM	1365	N	SER		437	-15.16		6.448		35.19	7
	ATOM	1366	CA	SER		437	-14.12		5.445		33.03	6
	ATOM	1367	CB	SER		437	-12.88		5.847		35.31	6
30	ATOM	1368	OG	SER			-11.85		4.879		44.99	8
	ATOM	1369	C			437	-14.64		4.108		38.39	6
	ATOM	1370	Ö			437	-14.70		3.127		37.54	8
	ATOM	1371	N			438	-15.00		4.096		37.32	7
	ATOM	1372	CA			438	-15.52		2.908		39.30	6
35	ATOM	1373	СВ			438	-16.01		3.259		42.97	6
	ATOM	1374	CG			438	-14.91		3.590		41.72	6
	MOTA	1375	CD			438	-14.04		2.356		45.23	6
	ATOM	1376	NE			438	-14.78		1.235		45.66	7
	ATOM	1377	CZ			438	-14.48		-0.040		49.71	6
40	ATOM	1378	NH1			438	-13.45		-0.347		50.91	7
	ATOM	1379		ARG			-15.21		-1.002		46.86	7
	ATOM	1380	С			438	-16.65				42.37	6
	ATOM	1381	0	ARG	В	438	-16.84		1.072	1.00	40.58	8
	ATOM	1382	N			439	-17.41				42.25	7
45	ATOM	1383	CA			439	-18.53		2.614		42.81	6
	ATOM	1384	СВ	PHE	В	439	-19.19		3.731		42.18	6
	ATOM	1385	CG			439	-20.48				42.48	6
	ATOM	1386		PHE	,		-21.53		2.912		47.09	6
	ATOM	1387		PHE			-20.63		3.334		39.76	6
50	ATOM	1388		PHE			-22.73		2.527		49.17	6
	ATOM	1389		PHE			-21.85		2.944		45.10	6
	ATOM	1390	CZ			439	-22.90		2.538		46.36	6
	ATOM	1391	С			439	-18.01		1.581		44.79	6
	ATOM	1392	ō .			439	-18.51		0.465		40.26	8
55	ATOM	1393	N			440	-17.02		1.987		42.77	7
	ATOM	1394	CA			440	-16.41		1.109		42.96	6
	ATOM	1395	СВ			440	-15.16		1.768		37.19	6
	ATOM	1396	CG			440	-15.47		2.967		36.97	6

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5	ATOM	1397		1 LEU			91.352	3.402	2 1.00 33.65	_
	ATOM	1398		2 LEU						
	ATOM	1399			B 440		88.561		•	
	ATOM	1400			B 440	-16.631				8
10	ATOM	1401			B 441	-15.238				7
10	ATOM	1402			B 441	-14.929				
	ATOM	1403		HIS	B 441	-14.150				6
	ATOM	1404		HIS		-12.713		-1.230		6
	ATOM	1405		2 HIS	B 441	-11.602		-1.812		6
	ATOM	1406		l HIS		-12.245		-0.273		6
15	ATOM	1407	CE	l HIS	B 441	-10.916		-0.309		7
	ATOM	1408	NE	2 HIS	B 441	-10.512		-1.228		6
	ATOM	1409	С	HIS	B 441	-16.217		-2.301		7
	ATOM	1410	0		B 441	-16.418		-3.465		6
	ATOM	1411	N		B 442	-17.106		-1.553		8
20	ATOM	1412	CA		B 442	-18.399		-2.106		7
	ATOM	1413	CB		B 442	-19.340				6
	ATOM	1414	CG		B 442	-18.991		-1.008	1.00 55.93	6
	ATOM	1415	SD		B 442	-20.310		-0.456	1.00 58.52	6
	ATOM	1416	CE	MET		-20.525		0.505	1.00 60.99	16
25	ATOM	1417	С		3 442	-18.991	86.879	1.827	1.00 52.61	6
	MOTA	1418	0		3 442	-19.646		-2.785	1.00 60.31	6
	ATOM	1419	N		3 443	-18.731	86.778 88.045	-3.817	1.00 58.18	8
	ATOM	1420	CA		3 443	-19.267	89.268	-2.213	1.00 61.45	7
	ATOM	1421	CB	LYS E		-19.182	90.358	-2.758	1.00 64.90	6
30	ATOM	1422	CG	LYS E		-20.160	90.338	-1.704	1.00 64.40	6
	ATOM	1423	CD	LYS E		-19.763	92.673	-1.982	1.00 69.12	6
	ATOM	1424	CE	LYS E		-20.508	92.993	-1.306	1.00 71.14	6
	ATOM	1425	NZ	LYS E		-20.174	94.242	-0.491	1.00 73.43	6
	ATOM	1426	С	LYS E		-18.528	89.704	0.151	1.00 67.97	7
35	ATOM	1427	0	LYS E		-18.979	90.586	-4.020	1.00 67.29	6
	ATOM	1428	N	VAL E		-17.383	89.075	-4.731	1.00 67.90	8
	MOTA	1429	CA	VAL B		-16.589	89.418	-4.285 -5.455	1.00 66.57	7
	ATOM	1430	CB	VAL B		-15.097	89.568	-5.082	1.00 64.76	6
	ATOM	1431	CG1	VAL B		-14.269	89.857	-6.298	1.00 62.76	6
40	ATOM	1432		VAL B		-14.905	90.678	-4.042	1.00 64.00	6
	ATOM	1433	С	VAL B		-16.800		-6.569	1.00 59.27	6
	ATOM	1434	0	VAL B		-16.968	88.774			6
	ATOM	1435	N	GLU B		-16.812	87.118	-7.729 -6.219	1.00 70.60	8
	ATOM	1436	CA	GLU B		-16.951	86.033		1.00 70.71	7
45	MOTA	1437	CB	GLU B		-16.169	84.809	-7.197	1.00 71.45	6
	MOTA	1438	CG	GLU B		-14.736		-6.712	1.00 72.36	6
	ATOM	1439	CD	GLU B		-13.998	85.090	-6.392	1.00 40.00	6
	ATOM	1440	OE1	GLU B		-14.587	83.890	-5.851	1.00 40.00	6
	ATOM	1441		GLU B		-12.775	82.798	-5.665	1.00 40.00	8
50	ATOM	1442		GLU B		-18.375	83.995	-5.580	1.00 40.00	8
	ATOM	1443		GLU B		-18.605	85.574	-7.422	1.00 71.46	6
	ATOM	1444		CYS B			84.542	-8.064	1.00 73.02	8
	ATOM	1445		CYS B		-19.328	86.333	-6.900	1.00 71.12	7
	ATOM	1446		CYS B		-20.694	85.942	-7.062	1.00 70.83	6
55	ATOM	1447		CYS B		-21.196	85.230	-5.784	1.00 71.05	6
	ATOM	1448		CYS B		-20.296	83.720	-5.349		16
	ATOM	1449		CYS B		-21.563	87.135	-7.386	1.00 71.91	6
	ATOM	1450				-21.307		-6.911	1.00 72.06	8
		1430	1.0	PRO B	44/	-22.550	86.928	-8.256	1.00 73.12	7

5	» mov	1451	CD F	PRO B	447	-22.837	85.637	-8.886	1.00 72.88	6
3	ATOM	1451		PRO B		-23.461		-8.653	1.00 74.22	6
	ATOM	1452		PRO B		-24.399	87.338	-9.659	1.00 72.98	6
	MOTA	1454		PRO B		-23.981	85.934	-9.776	1.00 74.77	6
	ATOM	1455		PRO B		-24.203	88.519	-7.451	1.00 75.94	6
10	MOTA	1456		PRO B		-24.601	87.749	-6.611	1.00 76.67	8
10	ATOM	1457		THR B		-24.390	89.828	-7.373	1.00 76.91	7
	MOTA	1457		THR B		-25.134	90.436	-6.268	1.00 78.24	6
	MOTA	1456		THR B		-24.883	91.948	-6.276	1.00 81.33	6
	ATOM			THR B		-25.474	92.525	-7.451	1.00 84.46	8
	MOTA	1460		THR B		-23.394	92.234	-6.269	1.00 83.51	6
15	MOTA	1461		THR B		-26.594	90.160	-6.619	1.00 77.42	6
	ATOM	1462		THR B		-27.512	90.649	-5.982	1.00 77.65	8
	ATOM	1463		GLU B		-26.759	89.400	-7.697	1.00 76.29	7
	MOTA	1464		GLU B		-28.051	89.017	-8.211	1.00 75.03	6
-00	MOTA	1465				-27.923	88.915	-9.719	1.00 74.62	6
20	MOTA	1466		GLU B		-28.823	87.966		1.00 40.00	6
	MOTA	1467				-28.523	87.831		1.00 40.00	6
	ATOM	1468		GLU B		-27.366	88.072		1.00 40.00	8
	MOTA	1469		GLU B		-29.449	87.438		1.00 40.00	8
0.5	ATOM	1470		GLU B		-28.448	87.660	-7.609	1.00 73.49	6
25	ATOM	1471	C	GLU B		-29.479	87.092	-7.953	1.00 70.24	8
	MOTA	1472	O N	LEU B		-27.624	87.158	-6.695	1.00 70.80	7
	ATOM	1473	N	LEU B		-27.879	85.879	-6.058	1.00 68.82	6
	ATOM	1474	CA	LEU B		-26.772	84.887	-6.447	1.00 71.91	6
20	ATOM	1475	CB CG	LEU B		-26.612	84.503	-7.900	1.00 76.62	6
30	ATOM	1476		LEU B		-25.396	83.637	-8.059	1.00 77.95	6
	ATOM	1477		LEU E		-27.849	83.775	-8.351	1.00 76.46	6
	ATOM	1478	CD2	LEU E		-27.941	86.012	-4.536	1.00 66.22	6
	ATOM	1479 1480	0	LEU E		-28.251	85.039	-3.849	1.00 66.01	8
35	ATOM	1480	N	PHE E		-27.666	87.215	-4.012	1.00 61.96	7
35	MOTA	1482	CA	PHE E		-27.635	87.494	-2.585	1.00 58.44	6
	MOTA	1482	CB	PHE E		-26.579	88.573	-2.263	1.00 61.34	6
	MOTA	1484	CG	PHE I		-25.153	88.078	-2.413	1.00 63.02	6
	ATOM	1485		PHE I		-24.675	87.587	-3.626	1.00 62.92	6
40	ATOM	1486		PHE I		-24.283		-1.346	1.00 63.07	6
40	ATOM	1487		PHE I		-23.327	87.217	-3.757	1.00 65.12	6
	ATOM	1488		PHE		-22.939		-1.472	1.00 64.66	6
	MOTA	1489			B 451	-22.459		-2.686		6
	ATOM ATOM	1490			B 451	-28.931		-1.962		6
45	ATOM	1491			B 451	-29.207		-1.908	1.00 56.56	8
43	ATOM	1492			B 452	-29.791		-1.473	1.00 53.28	7
	MOTA	1493			B 452	-29.767		-1.494	1.00 50.46	6
		1494			B 452	-31.037				6
	ATOM	1495			B 452	-31.746			1.00 49.19	6
50	ATOM ATOM	1496			B 452	-31.024				6
30	ATOM	1497			B 452	-30.636			1.00 49.62	6
	ATOM	1498			B 452	-29.628				8
		1499			B 453	-31.494				7
	ATOM ATOM	1500			B 453	-32.853				6
55		1500			B 453	-31.184				6
33	ATOM	1502			B 453	-32.422			1.00 51.49	6
	ATOM	1502			B 453	-33.378			1.00 50.82	6
	MOTA	150			B 453	-30.829				6
	ATOM	150.		110	J 433	JJ.J2.				

5	ATOM	1505	0			453	-29.700	90.206	3.345	1.00	54.17	8
	MOTA	1506	N	LEU	В	454	-31.807	89.458	3.631	1.00	51.21	7
	ATOM	1507	CA	LEU	В	454	-31.538	88.945	4.948		47.17	6
	ATOM	1508	CB	LEU	В	454	-32.550	87.858	5.330		44.44	6
	ATOM	1509	CG			454	-32.347	87.412	6.748		41.33	6
10	ATOM	1510	CD1				-31.987	88.589	7.631		35.93	6
	ATOM	1511	CD2			454	-33.590	86.732	7.239		34.79	
	ATOM	1512	С			454	-30.099	88.443	4.928			6
	ATOM	1513	Ō			454	-29.323	88.774			42.25	6
	ATOM	1514	N			455	-29.716		5.812		40.82	8
15	ATOM	1515	CA			455	-28.347	87.707	3.885		39.29	7
	ATOM	1516	CB			455		87.204	3.770		41.81	6
	ATOM	1517	CG			455	-28.132	86.536	2.418		47.22	6
	ATOM	1518					-26.813	85.836	2.292		56.97	6
	ATOM		CD1			455	-26.437	84.915	3.247		57.23	6
20		1519	CD2				-25.949	86.094	1.236		59.40	6
20	ATOM	1520	CE1				-25.225	84.234	3.153		56.58	6
	ATOM	1521	CE2				-24.720	85.409	1.134	1.00	61.80	6
	ATOM	1522	CZ	PHE			-24.360	84.481	2.103	1.00	59.94	6
	ATOM	1523	С	PHE			-27.400	88.386	3.923	1.00	45.12	6
25	ATOM	1524	0	PHE			-26.657	88.450	4.889	1.00	39.95	8
25	MOTA	1525	N	LEU	- 4		-27.439	89.303	2.949	1.00	43.92	7
	ATOM	1526	CA	LEU			-26.597	90.503	2.947	1.00	44.08	6
	ATOM	1527	CB	LEU			-27.001	91.440	1.802	1.00	50.20	6
	MOTA	1528	CG	LEU			-26.439	91.155	0.432	1.00	55.79	6
20	ATOM	1529		LEU			-27.064	92.082	-0.591	1.00	54.70	6
30	ATOM	1530	CD2	•			-24.920	91.345	0.494	1.00	53.01	6
	ATOM	1531	С	LEŲ			-26.689	91.245	4.264	1.00	44.65	6
	ATOM	1532	0	LEU			-25.678	91.540	4.886	1.00	45.93	8
	ATOM	1533	N	GLU			-27.990	91.268	4.265	1.00	44.56	7
25	ATOM	1534	CA	GLU			-28.288	92.016	5.497	1.00	46.37	6
35	ATOM	1535	С	GLU			-27.434	91.452	6.628	1.00	43.60	6
	ATOM	1536	0	GLU	•		-26.754	92.223	7.339	1.00	42.69	8
	ATOM	1537	CB	GLU			-29.769	91.879	5.855	1.00	50.16	6
	ATOM	1538	CG	GLU			-30.208	92.849	6.954	1.00	20.00	6
	ATOM	1539	CD	GLU	В	457	-31.646	93.338	6.782		20.00	6
40	ATOM	1540	OE1	GLU		457	-32.351	92.932	5.779		20.00	8
•	MOTA	1541	OE2	GLU	В	457	-32.157	94.156	7.638		20.00	8
	ATOM	1542	N	VAL	В	458	-27.428	90.413	7.281	-	43.21	7
	ATOM	1543	CA	VAL	В	458	-26.706	89.739	8.351		44.98	6
	ATOM	1544	CB	VAL	В	458	-27.075	88.255	8.432		44.83	6
45	ATOM	1545	CG1	VAL	Ė	458	-26.440	87.623	9.646		49.72	6
	ATOM	1546	CG2	VAL	Ė	458	-28.562	88.086	8.474		40.89	6
	MOTA	1547	С	VAL			-25.190	89.822	8.311		42.72	6
	ATOM	1548	0	VAL	-		-24.551	90.179	9.303		42.88	8
	ATOM	1549	N	PHE			-24.605	89.488	7.180		44.53	7
50	ATOM	1550	CA	PHE			-23.165	89.480	7.077		48.18	
	ATOM	1551	СВ	PHE			-22.747	88.457	6.065		43.60	6
	ATOM	1552	CG	PHE			-23.167	87.116				6
	ATOM	1553		PHE			-24.494		6.441		40.79	6
	ATOM	1554		PHE			-22.263	86.750	6.368		41.01	6
55	ATOM	1555		PHE				86.286	7.009		39.48	6
	ATOM	1556		PHE			-24.892	85.540	6.889		40.62	6
	ATOM	1557	CZ	PHE			-22.649	85.091	7.527		36.87	6
	ATOM	1558	C	PHE			-23.967	84.711	7.455		36.39	6
	111 011	1330	C	FUF	D	409	-22.627	90.758	6.623	1.00	52.71	6

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					450		-21.414	91.050	6.791	1.00 51.34	8
5	MOTA	1559		PHE B				91.531		1.00 62.92	7
	MOTA	1560		GLU B			-23.489	92.741	5.533	1.00 69.33	6
	ATOM	1561		GLU B			-22.953	93.487	4.505	1.00 72.95	6
	ATOM	1562		GLU B			-23.851		3.412	1.00 78.35	6
	MOTA	1563		GLU B			-22.917	94.002	3.256	1.00 82.97	6
10	ATOM	1564		GLU E			-22.908	95.480		1.00 88.28	8
	MOTA	1565		GLU E			-23.257	96.213	4.217	1.00 84.80	8
	ATOM	1566	OE2	GLU E	460		-22.524	95.977	2.167	1.00 34.00	6
	ATOM	1567	С	GLU E	3 460		-22.790	93.576	6.786		8
	ATOM	1568	0	GLU E	3 460		-23.471	93.391	7.802	1.00 74.51	7
15	ATOM	1569		ASP F			-21.796	94.449	6.696	1.00 78.50	
13	ATOM	1570	CA		3 461		-21.401	95.328	7.701	1.00 84.19	6
	ATOM	1571	СВ		3 461		-20.182	96.032	7.125	1.00 85.82	6
	ATOM	1572	CG		в 461		-19.261	95.066	6.463	1.00 89.62	6
	ATOM	1573			в 461		-19.670	93.929	5.982	1.00 93.00	8
20	ATOM	1574			в 461		-18.084	95.361	6.387	1.00 93.04	8
20	ATOM	1575	C		B 461		-22.540	96.291	8.012	1.00 86.80	6
		1576	0		B 461		-23.063	96.176	9.139	1.00 88.70	8
	ATOM	1577			B 461		-22.962	97.048	7.098	1.00 88.70	8
	ATOM	1311	OAI	1101			_				
25	TER	4002	C1	т3	J 1		20.152	36.643	29.561	1.00 22.34	6
25	MOTA	4002	C2	т3			19.021	41.567	29.283	1.00 21.84	6
	MOTA	4003	C3	T3	J 1 J 1		18.880	37.086	29.226	1.00 23.43	6
	ATOM	4004	C4	Т3	J 1		18.249	42.606	28.776	1.00 22.31	6
	ATOM	4005	C5	Т3	J 1		18.747	38.372	28.866	1.00 24.83	6
20	MOTA	4000	C6	Т3	J 1		17.938	43.621	29.664	1.00 25.16	6
30	MOTA	4007		T3			19.799	39.296	28.753	1.00 24.65	6
	ATOM	4008		T3	.T 1		18.330	43.594	31.028	1.00 21.93	6
	ATOM	4009		T3	\ddot{J} 1	•	21.101		29.075	1.00 25.09	6
	ATOM	4010		T3	J 1		19.063		31.465	1.00 23.66	6
2.5	MOTA	4011		1 T3	j " 1		21.254		29.456	1.00 23.12	6
35	ATOM				J : 1		19.459		30.621	1.00 19.67	6
	ATOM	4013 4014			J		20.370		30.075	1.00 18.97	6
	ATOM				J		21.549		29.455	1.00 19.32	6
	ATOM	4015				1	21.535		29.710	1.00 19.02	6
	MOTA	4016		7 13 T3		1	16.898		28.661	1.00 25.29	53
40	ATOM	4017		T3		1	17.058		29.154	1.00 26.49	53
	MOTA	4018		Т3		1	22.763		29.169	1.00 25.67	53
	MOTA	4019				1	21.800		28.024	1.00 15.12	7
	ATOM	4020				1	17.93		31.806	1.00 21.79	8
	MOTA	402				1	19.43		28.362	1.00 22.05	8
45						1	21.91		28.776	1.00 20.38	8
	ATOM				J	1	21.13		30.840		8
	MOTA	402	4 04	Т3	J	1	21.13	, 32.322			
	TER		1	m a	17	1	-28.13	1 75.928	7.543	3 1.00 22.34	6
	MOTA				K	1			4.318		6
50					K	1	-24.67 -28.49		6.20		
	ATOM				K	1	-28.49 -24.21		2.98		
	ATOM				K	1			5.23		
	ATOM				K	1	-27.48		2.70		
	ATOM				K	1	-23.54				
5.5	5 ATOM				K	1	-26.13			00	6
	ATOM				K	1	-23.38		_		6
	MOTA					1	-25.68				6
	MOTA	403	34 C	10 T3	K	1	-23.86	79.823	5.04	2 1.00 20.00	_

_											
5	ATOM	4035	C1	1 T3	K	1	-26.70	8 75.670	7.834	1.00 23.12	_
	ATOM	4036	C1:	2 T3	K		-24.52				6
	ATOM	4037	C1:	3 T3	K		-29.21				6
	ATOM	4038		5 тз	K		-29.18				6
	ATOM	4039		7 T3	K	_	-30.44		-		6
10	ATOM	4040		T3	ĸ	_					6
	ATOM	4041		T3	K		-27.86				53
	ATOM	4042		T3			-22.73				53
	ATOM	4043			K		-23.60			1.00 25.67	53
	ATOM			T3	K		-28.68		8.762	1.00 15.12	7
15		4044		Т3	K		-22.742		3.443		8
13	ATOM	4045		Т3	K	_	-25.26	7 76.388	4.595		8
	ATOM	4046		Т3	K	1	-30.81	73.159			8
	ATOM	4047	04	Т3	K	1	-31.028	75.359			8
	TER									1.00 20.10	o
•	ATOM	1	С	LYS	X	686	13.868	40.176	48.888	1.00 40.00	_
20	ATOM	2	0	LYS	Х	686	13.914	-			6
	ATOM	3	N			686	14.374				8
	ATOM	4	CA			686	14.937				7
	ATOM	5	N	HIS			13.038		49.710	1.00 40.00	6
	ATOM	6	CA	HIS			11.891		49.705	1.00 40.00	7
25	ATOM	7	СВ	HIS			10.639		49.521	1.00 40.00	6
	ATOM	8	CG	HIS					50.212	1.00 40.00	6
	ATOM	9		HIS			10.981		51.563	1.00 40.00	6
	ATOM	10		HIS			11.021		52.753	1.00 40.00	6
	ATOM	11		HIS			11.354		51.754	1.00 40.00	7
30	ATOM	12					11.614		53.034	1.00 40.00	6
	ATOM	13		HIS			11.422		53.646	1.00 40.00	7
	ATOM		С	HIS			11.183		48.208	1.00 40.00	6
	ATOM	14	0	HIS			11.674		47.094	1.00 40.00	8
	ATOM	15	N	LYS			10.064	37.458	48.649	1.00 40.00	7
35		16	CA	LYS			8.911	36.858	47.931	1.00 40.00	6
33	ATOM	17	CB	LYS			8.292	37.850	46.968	1.00 40.00	6
	ATOM	18	С	LYS			9.246	35.573	47.161	1.00 40.00	6
	ATOM	19	0	LYS			9.319	34.473	47.722	1.00 40.00	8
	ATOM	20	N	ILE	X	689	9.426	35.754	45.865	1.00 40.00	7
40	ATOM	21	CA	ILE	X	689	9.661	34.640	44.924	1.00 40.00	6
40	ATOM	22	CB	ILE	Х	689	9.731	35.167	43.498	1.00 40.00	
	ATOM	23	CG2	ILE	Х	689	9.638	34.053	42.453	1.00 40.00	6
	ATOM	24	CG1	ILE	X	689	8.597	36.141	43.176		6
	ATOM	25		ILE			8.250	36.183	41.688	1.00 40.00	6
	ATOM	26	С	ILE			10.954	33.869		1.00 40.00	6
45	ATOM	27	0	ILE			10.920	32.657	45.228	1.00 40.00	6
	ATOM	28	N	LEU			12.065		45.511	1.00 40.00	8
	ATOM	29	CA	LEU :			13.391	34.579	45.140	1.00 40.00	7
	ATOM	30	СВ	LEU				33.996	45.397	1.00 40.00	6
	ATOM	31	CG	LEU			14.349	35.043	45.892	1.00 40.00	6
50	ATOM	32		LEU :			14.450	36.168	44.906	1.00 40.00	6
	ATOM	33	CDI	LEU .	X (590	15.397	37.261	45.363	1.00 40.00	6
	ATOM			LEU :			14.940	35.695	43.540	1.00 40.00	6
	ATOM	34		LEU 2			13.271	32.999	46.466	1.00 40.00	6
		35		LEU >			13.633	31.832	46.315	1.00 40.00	8
55	ATOM	36		HIS >			12.773	33.472	47.541	1.00 40.00	7
55	ATOM	37		HIS >			12.557	32.559	48.569	1.00 40.00	
	ATOM	38		HIS >			11.729	33.212	49.658	1.00 40.00	6
	ATOM	39		HIS >			12.588	34.116	50.564	1.00 40.00	6
	ATOM	40		HIS >			13.648	33.852	51.385	1.00 40.00	6
								33.032	51.505	1.00 40.00	6

			12 359 35.484 50.669 1.00 40.00 7
5	ATOM	41 ND1 HIS X 691	12.359 33.464 30.663 1.00 40.00 6
,	ATOM	42 CE1 HIS X 691	13.242 33.331 32.32
	MOTA	43 NE2 HIS X 691	14.016 35.031 31.545 21.00 40 00 6
	MOTA	44 C HIS X 691	11.954 31.331 47.331
	ATOM	45 O HIS X 691	12.505 30.240 47.662 1.00 40 00 7
10	ATOM	46 N ARG X 692	10.839 31.494 47.107 1.00 40 00 6
10	ATOM	47 CA ARG X 692	10.169 30.333 40.310 1.00 40 00 6
	ATOM	48 CB ARG X 692	9.118 30.800 45.517 1.00 40.00 6
	ATOM	49 C ARG X 692	11.153 29.402 45.752 2.00
	ATOM	50 O ARG X 692	11.030 28.166 45.775 1.00 10.00
15	ATOM	51 N LEU X 693	12.11/ 30.000 45.072 1.00
13	ATOM	52 CA LEU X 693	13.078 29.252 44.220 1.00
	ATOM	53 CB LEU X 693	13.784 30.210 43.274 200
	ATOM	54 CG LEU X 693	12.796 31.012 42.432 1.00
	MOTA	55 CD1 LEU X 693	13.4/9 31.909 41.430
20	ATOM	56 CD2 LEU X 693	11.884 30.120 41.373
20	ATOM	57 C LEU X 693	14.143 28.551 45.054 10.00 8
	ATOM	58 O LEU X 693	14.702 27.508 44.055 110
	ATOM	59 N LEU X 694	14.400 29.079 40.203 1.00 10.00
	MOTA	60 CA LEU X 694	15.407 28.550 47.115 1.00
25	MOTA	61 CB LEU X 694	15.8/1 29.620 40.00 6
23	ATOM	62 CG LEU X 694	16.692 30.710 47.101
	ATOM	63 CD1 LEU X 694	17.279 31.724 40.332 200
	ATOM	64 CD2 LEU X 694	17.879 30.130 40.025
	ATOM	65 C LEU X 694	14.837 27.404 47.55
30	ATOM	66 O LEU X 694	15.555 26.747 40.715 20.40.00 7
50	ATOM	67 N GLN X 695	13.554 27.157 47.005 2.00
	ATOM	68 CA GLN X 695	12.883 26.188 40.003 1.00 40.00 6
	MOTA	69 C GLN X 695	12.425 24.515 10.40.00 8
	ATOM	70 O GLN X 695	12.309 23.645 40.330 1.00 40 00 6
35		71 CB GLN X 695	11.681 26.636 49.322 200
55	ATOM	72 CG GLN X 695	12.074 20.125 50.000 1 00 20 00 6
	ATOM	73 CD GLN X 695	10.899 20.700 50.002 210
	MOTA	74 OE1 GLN X 695	9.772 20.290 30.072 20.00 7
	MOTA	75 NE2 GLN X 695	11.092 29.828 31.300 1.00 40.00 7
40		76 N ASP X 696	12.155 25.020 40.714 1.00 40.00 6
	ATOM	77 CA ASP X 696	11.698 23.883 43.313
	ATOM	78 CB ASP X 696	11.450 24.400 44.497 1.00.10.00
	ATOM	79 CG ASP X 696	10.782 23.411 43.310 2100 40 00 8
	ATOM	80 OD1 ASP X 696	10.550 22.203 43.323 1 00 40 00
4:		81 OD2 ASP X 696	10.449 23.804 42.302 1 00 40 00 6
	MOTA	82 C ASP X 696	12.774 22.000 1 00 10 00 8
	MOTA	83 O ASP X 696	13.937 23.077 43.332 100 40 00 7
	ATOM	84 N SER X 697	12.370 21.610 46.213
	ATOM	85 CA SER X 697	13.258 20.433 40.120 2100 40.00 6
5	MOTA 0	86 CB SER X 697	12.685 19.371 47.073
	MOTA	87 OG SER X 697	12.555 15.655 1 00 40 00 6
	ATOM	88 C SER X 697	13.323 20.23
	ATOM	89 O SER X 697	14.24, 20.00
	ATOM	90 N SER X 698	12.333 13.30
5	55 ATOM	91 CA SER X 698	11.903 13.10
_	MOTA	92 CB SER X 698	11.693 20.417 42.555 1.00 40 00 8
	MOTA	93 OG SER X 698	10.310 22.000
	ATOM	94 C SER X 698	12.887 18.340 41.758 1.00 40.00 6

£	7 MOM	٥٤		SER X 6	00	13.253	17.158	42.026	1.00 4	10.00	8
5	ATOM	95 96		SER X 6		13.131	18.976	40.714	1.00 4		8
	ATOM	90	OXI .	SER A C	, , 0	13.131	10.00	••••			-
	TER ATOM	1	СВ :	LYS Y 6	9.9	-33.793	96.885	6.491	1.00	40.00	6
		2		LYS Y 6		-35.002	95.370	8.130	1.00		6
10	ATOM	3		LYS Y 6		-36.027	95.520	8.779	1.00		8
10	ATOM	3 4			588	-32.717	96.619	8.695	1.00		7
	ATOM	5			588	-34.040	96.591	7.954	1.00		6
	ATOM	6			589	-34.578	93.781	6.908	1.00		7
	ATOM	7			589	-35.862	93.106	7.268	1.00		6
15	ATOM	8			689	-35.971	91.759	6.572	1.00		6
15	MOTA	9			689	-37.270	91.077	6.932		40.00	6
	MOTA			ILE Y		-35.917	91.937	5.062		40.00	6
	ATOM	10		ILE Y		-36.341	90.691	4.289		40.00	6
	ATOM	11	CDI	ILE Y		-36.032	92.870	8.780		40.00	6
20	ATOM	12	0	ILE Y		-36.913	93.446	9.442		40.00	8
20	ATOM	13		LEU Y		-35.019	92.834	9.787		40.00	7
	ATOM	14		LEU Y		-34.956	92.320	11.163		40.00	6
	ATOM	15 16	CA CB	LEU Y		-33.528	92.432	11.697		40.00	6
	ATOM	17	CG	LEU Y		-32.516	91.647	10.864		40.00	6
25	ATOM	18		LEU Y		-31.087	91.764	11.397		40.00	6
25	ATOM	19		LEU Y		-32.819	90.148	10.812		40.00	6
	MOTA	20	CDZ	LEU Y		-35.899	93.123	12.065		40.00	6
	ATOM	21	0	LEU Y		-36.570	92.492	12.928		40.00	8
	ATOM ATOM	22	N		691	-36.039	94.731	11.373		40.00	7
30	ATOM	23	CA		691	-36.634	94.923	12.683		40.00	6
30	ATOM	24	CB	HIS Y		-36.054	96.383	12.935		40.00	6
	ATOM	25	CG	HIS Y		-35.610	97.153	13.078		40.00	6
	ATOM	26		HIS Y		-34.757	97.640	12.159	1.00	40.00	6
	ATOM	27		HIS Y		-35.129	97.579	14.319	1.00	40.00	7
35	ATOM	28		HIS Y		-34.039	98.290	14.122	1.00	40.00	6
55	ATOM	29		HIS Y		-33.786	98.346	12.815	1.00	40.00	7
	ATOM	30	C	HIS Y		-37.972	94.287	12.756	1.00	40.00	6
	ATOM	31	Ō	HIS Y		-38.240	93.417	13.545	1.00	40.00	8
	ATOM	32	N	ARG Y		-38.265	94.388	11.505	1.00	40.00	7
40	ATOM	33	CA	ARG Y		-39.577	93.869	11.276	1.00	40.00	6
	ATOM	34	СВ	ARG Y		-39.653	93.692	9.795	1.00	40.00	6
	ATOM	35	CG	ARG Y		-40.759	92.764	9.329	1.00	40.00	6
	MOTA	36		ARG Y		-40.618	92.422	7.848		40.00	6
	MOTA	37		ARG Y	692	-41.849	92.641	7.091		40.00	7
45	ATOM	38		ARG Y	692	-41.898	92.758	5.763		40.00	6
	ATOM	39		ARG Y	692	-40.784	92.695	5.024		40.00	7
	ATOM	40		ARG Y	692	-43.034	92.940	5.080		40.00	7
	ATOM	41		ARG Y	692	-39.941	92.547	11.995		40.00	6
	MOTA	42		ARG Y		-41.001	92.440	12.649		40.00	8
50	MOTA	43		LEU Y	693	-39.095	91.576	11.816	1.00	40.00	7
	ATOM	44		LEU Y	693	-39.230	90.232	12.395	1.00	40.00	6
	ATOM	45	СВ	LEU Y	693	-38.362	89.337	11.615	1.00	40.00	6
	ATOM	46		LEU Y	693	-38.737	89.375	10.132	1.00	40.00	6
	ATOM	47				-37.794	88.570	9.247		40.00	6
55		48		LEU Y		-40.142	88.827	9.862		40.00	6
	ATOM	49		LEU Y	693	-38.921	90.378	13.816		40.00	6
	ATOM	50		LEU Y		-39.191	89.474	14.615		40.00	8
	ATOM	51		LEU Y		-38.366	91.533	14.076	1.00	40.00	7

5	ATOM	52	CA	LEU	Y	694	-38.174	91.885	15.435	1 00	40.00	_
	ATOM	53	CB	LEU		694	-37.181	93.002	15.561		40.00	6
	ATOM	54	CG	LEU			-35.799	92.377	15.869			6
	ATOM	55	CD1	LEU	_		-34.897	93.275	16.702		40.00	6
	ATOM	56	CD2				-35.897	91.055			40.00	6
10	ATOM	57	C	LEU	-		-39.596		16.661		40.00	6
	ATOM	58	0	LEU			-39.985	91.903	15.915		40.00	6
	ATOM	59	N	GLN	_	695	-40.787	91.253	16.858		40.00	8
	ATOM	60	CA	GLN	_	695		92.229	15.048		40.00	7
	ATOM	61	C	GLN	_		-42.034	91.457	15.543		40.00	6
15	ATOM	62	-				-43.054	90.901	14.240		40.00	6
15	ATOM		0	GLN			-43.102	91.557	13.189	1.00	40.00	8
	ATOM	63	CB	GLN		695	-42.362	92.025	16.923	1.00	40.00	6
		64	CG	GLN			-41.013	92.101	17.768	1.00	40.00	6
	ATOM	65	CD	GLN	_	695	-40.943	91.235	19.059	1.00	40.00	6
20	ATOM	66	OE1	GLN	-	695	-41.828	90.426	19.318	1.00	40.00	8
20	ATOM	67	NE2	GLN	Y	695	-39.938	91.399	19.916	1.00	40.00	7
	ATOM	68	N	ASP	Y	696	-43.802	89.498	14.402		40.00	7
	ATOM	69	CA	ASP	Y	696	-44.784	88.354	13.428		40.00	6
	ATOM	70	С	ASP	Y	696	-46.034	88.934	12.759		40.00	6
	ATOM	71	0	ASP	Y	696	-46.266	88.655	11.529		40.00	8
25	ATOM	72	CB	ASP	Y	696	-45.211	87.192	14.322		40.00	6
	ATOM	73	CG	ASP	Y	696	-44.021	86.560	15.058		40.00	6
	ATOM	74	OD1	ASP	Y	696	-42.823	86.994	14.844		40.00	8
	ATOM	75	OD2	ASP	Y	696	-44.212	85.591	15.889		40.00	8
	END						• • • • • • • • • • • • • • • • • • • •		10.005	1.00	40.00	0
30												

Appendix 2

Atomic Coordinates for Human ERa Complexed with DES, and a GRIP1 NR-box 2 Peptide

10	CRYST1	54.	094 8	2.217	58.	041	90.00	1:	11.33	90.00	P 21	2
	ORIGX1	1.	000000	0.00	0000	0	.000000	0	.00000			
	ORIGX2	0.	000000	1.00	0000		.000000		.00000			
	ORIGX3	0.	000000	0.00	0000		.000000		.00000			
	SCALE1		018486		0000		.007221		.00000			
15	SCALE2	0.	000000	0.01	2163		.000000		.00000			
	SCALE3	0.	000000	0.00			.018497		.00000			
	ATOM ATOM	1	СВ	SER	A	305	35	.230	-14.78	7 -1.163	1,00	73.26
20	ATOM	2 3	C	SER	A	305			-14.303		1.00	72.95
	ATOM	4	O	SER	A	305			-13.984		1.00	72.46
	ATOM	5	N	SER	A	305			-16.033		1.00	74.06
	ATOM	6	CA N	SER	A	305			-14.713		1.00	73.59
	ATOM	7		LEU	A	306					1.00	72.21
25	ATOM	8	CA CB	LEU	A	306			-13.950		1.00	71.05
	ATOM	9	C	LEU	A	306		.251	-14.256		1.00	70.19
	ATOM	10	0	LEU	A	306		.929	-12.478		1.00	69.57
	ATOM	11	N	LEU	A	306			-11.638		1.00	69.96
	ATOM	12	CA	ALA ALA	. A	307		.851	-12.176		1.00	68.06
30	ATOM	13	CB	ALA ALA	A	307		.358	-10.810		1.00	64.88
	ATOM	14	C	ALA	. A	307		.841	-10.795		1.00	65.83
	ATOM	15	0	ALĄ	A A	307		.792	-10.204		1.00	63.36
	ATOM	16	N	LEU	A	307		.878	-8.984		1.00	62.73
	ATOM	17	CA	LEU	A	308		.064	-11.062		1.00	62.52
35	ATOM	18	CB	LEU	A	308		.487	-10.598		1.00	62.57
	ATOM	19	CG	LEU	A	308 308		.423	-11.745		1.00	62.81
	ATOM	20	CD1	LEU	A	308		.214	-12.688		1.00	64.21
	ATOM	21	CD2	LEU	A	308		188		10.406	1.00	66.28
	MOTA	22	C	LEU	A	308		919	-11.898		1.00	63.80
40	ATOM	23	ō	LEU	A	308		903	-10.037		1.00	61.61
	ATOM	24	N	SER	A	309		385	-9.445		1.00	62.92
	ATOM	25	CA	SER	A	309		561	-10.219		1.00	60.50
	ATOM	26	CB	SER	A	309		928	-9.743		1.00	58.73
	ATOM	27	OG	SER	A	309		720 889	-10.750		1.00	59.53
45	ATOM	28	С	SER	A	309		986	-10.283		1.00	59.47
	ATOM	29	0	SER	A	309		965	-8.373	6.099	1.00	57.05
	ATOM	30	N	LEU	A	310		940	-7.637	6.249	1.00	56.70
	ATOM	31	CA	LEU	A	310		877	-8.038 -6.759	5.352	1.00	52.69
	ATOM	32	CB	LEU	A	310		516			1.00	48.20
50	ATOM	33	CG	LEU	A	310		301	-6.596	3.974	1.00	48.32
	ATOM	34	CD1	LEU	A	310		951	-7.188	2.583	1.00	44.94
	ATOM	35	CD2	LEU	A	310		417	-6.728	2.055	1.00	46.45
	ATOM	36	С	LEU	A	310		086	-6.755	1.650	1.00	43.19
	ATOM	37	0	LEU		310		605	-5.589	5.609	1.00	46.44
55	ATOM	38	N	THR		311			-5.607	6.741	1.00	46.78
	ATOM	39	CA	THR		311	37. 38.		-4.576	5.148	1.00	44.36
	ATOM	40	CB	THR		311	39.		-3.380	5.949	1.00	42.88
	ATOM	41	OG1	THR		311	39. 39.		-2.633	5.532	1.00	42.31
	ATOM	42	CG2	THR		311	40.		-1.936	4.303	1.00	42.50
60	ATOM	43	C	THR		311	36.		-3.606	5.350	1.00	46.02
							٠٥.	034	-2.475	5.674	1.00	43.21

							26 021	-2.776	4.800	1.00 4	12.12
5	MOTA	44		-	A	311	36.021	-1.372	-		12.16
	ATOM	45		-	A	312	36.726	-0.444			40.10
	ATOM	46	CA	ALA	A	312	35.616	0.709			40.07
	MOTA	47	CB	ALA	A	312	35.741	0.709			41.80
	ATOM	48	С	ALA	A	312	35.561		4.154		37.81
10	ATOM	49	0	ALA	Α	312	34.510	0.074	4.134		42.35
	MOTA	50	N	ASP	Α	313	36.698	0.564	2.953		42.27
	ATOM	51	CA	ASP	Α	313	36.752	1.104			43.74
	MOTA	52	CB	ASP	Α	313	38.133	1.703	2.680		46.62
	MOTA	53	CG	ASP	Α	313	38.323	3.054	3.348		51.01
15	ATOM	54	OD1	ASP	Α	313	39.414	3.645	3.205	1.00	48.89
13	ATOM	55	OD2	ASP	Α	313	37.380	3.529	4.015	1.00	38.68
	ATOM	56	С	ASP	Α	313	36.422	0.027	1.926	1.00	38.75
	ATOM	57	Ō	ASP	Α	313	35.704	0.281	0.959	1.00	
	ATOM	58	N	GLN	Α	314	36.931	-1.179	2.145	1.00	34.76
20	ATOM	59	CA	GLN	Α	314	36.666	-2.277	1.229	1.00	33.55
20	ATOM	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	36.90
		61	CG	GLN	A	314	38.963	-3.384	1.436	1.00	40.45
	MOTA	62	CD	GLN	A	314	39.700	-4.610	1.905	1.00	43.13
	MOTA	63	OE1	GLN	Α	314	39.394	-5.196	2.935	1.00	43.60
25	MOTA	64	NE2	GLN	Α	314	40.701	-5.032	1.117	1.00	44.03
25	MOTA	65	C	GLN	A	314	35.176	-2.595	1.201	1.00	34.95
	ATOM		0	GLN	A	314	34.605	-2.860	0.140	1.00	32.89
	MOTA	66	N	MET	A	315	34.542	-2.564	2.374	1.00	32.54
	ATOM	67	CA	MET	Α	315	33.115	-2.848	2.470	1.00	35.46
	MOTA	68	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
30	MOTA	69		MET	A	315	31.137	-2.777	4.097	1.00	39.42
	MOTA	70	CG	MET	A	315	30.443	-4.426	4.053	1.00	46.55
	MOTA	71	SD		A	315	31.351	-5.205	5.397	1.00	45.29
	MOTA	72	CE	MET		315	32.311	-1.859	1.640	1.00	31.83
	MOTA	73	C	MET	A	315	31.453	-2.247	_	1.00	32.10
35	MOTA	74	0	MET	A	316	32.587			1.00	32.62
	MOTA	75	N	LAV	A	316	31.882			1.00	31.09
	MOTA	76	CA	VAL	A		32.395			1.00	34.77
	MOTA	77	CB	VAĻ	A	316 316	31.786			1.00	34.10
	ATOM	78	CG1	VAL	A	316	32.021				34.40
40	ATOM	79	CG2	VAL	A		32.092		-0.414	1.00	33.48
	ATOM	80	С	VAL	A	316	31.145		-1.200		32.49
	ATOM	81	0	VAĻ	A	316	33.337		7 -0.795		33.49
	MOTA	82	N	SER	À	317	33.682		-2.187		32.88
	MOTA	83	CA	SER	A		35.165		5 -2.297		35.77
45		84	CB	SER	A		35.825		7 -3.154		
	ATOM	85	OG	SER			32.849		5 -2.801		
	MOTA	86	С	SER					8 -3.880		
	MOTA	87	0	SER			32.279		9 -2.11		
	ATOM	88	N	ALĀ			32.792	_	6 -2.580		
50	MOTA (89	CA	ALA			32.03		1 -1.579		
	MOTA	90	CB	ALA	. A		32.15		5 -2.77		
	ATOM	91	С	ΑLĄ	. A		30.56		5 -2.77		
	ATOM	92	0	ALA	A	318	29.96		2 -3.784		
	MOTA	93	N	LEU	A	319	29.99		4 -1.79		
55		94	CA	LEU	T A	319	28.59		2 -1.86		
٥.	ATOM	95	СВ	LEU	J A	319	28.17		6 -0.54		
	ATOM	96	CG	LEU		319	28.07				
	MOTA	97				319	27.52				
	ATOM	98				319	27.19		3 0.24		
6				LE		A 319	28.34		7 -3.02	0 1.00	
O.	ATOM ATOM			LE		A 319	27.43	0 -1.47	5 -3.81	8 1.0	0 35.23
	AIOM		- •								

5	30014									
3	ATOM	101	N	LEU	A	320	29.140	-0.195 -3.120	1.00	32.53
	ATOM	102	CA	LEU	Α	320	28.972	0.756 -4.212	1.00	35.33
	ATOM	103	CB	LEU	A	320	30.052	1.839 -4.155	1.00	33.52
	ATOM	104	CG	ΓÉΩ	A	320	29.974	2.899 -3.054	1.00	34.60
	ATOM	105	CD1	LEU	Α	320	31.060	3.940 -3.292	1.00	33.69
10	ATOM	106	CD2	LEU	Α	320	28.611	3.562 -3.044	1.00	31.05
	ATOM	107	С	LEU	A	320	29.052	0.040 -5.561	1.00	
	ATOM	108	0	LEU	A	320	28.230	0.271 -6.446		35.41
	ATOM	109	N	AASP		321	30.042	-0.833 -5.720	1.00	39.16
	ATOM	110	N	BASP		321			0.50	36.33
15	ATOM	111	CA	AASP			30.041	-0.839 -5.695	0.50	35.76
	ATOM	112	CA	BASP		321	30.214	-1.559 -6.977	0.50	37.71
	ATOM	113	CB		A	321	30.258	-1.595 -6.925	0.50	37.11
	ATOM			AASP	A	321	31.537	-2.334 -6.973	0.50	40.01
		114	CB	BASP		321	31.573	-2.374 -6.826	0.50	39.41
20	ATOM	115	CG	AASP		321	31.694	-3.230 -8.195	0.50	41.93
20	ATOM	116	CG	BASP	Α	321	32.770	-1.562 -7.284	0.50	39.96
	ATOM	117	OD1	AASP	Α	321	31.523	-2.733 -9.329	0.50	42.11
	ATOM	118	OD1	BASP	Α	321	33.312	-1.868 -8.366	0.50	43.41
	ATOM	119	OD2	AASP	Α	321	31.988	-4.432 -8.022	0.50	42.69
	ATOM	120	OD2	BASP	A	321	33.170	-0.622 -6.564	0.50	41.33
25	MOTA	121	С	AASP	À	321	29.069	-2.524 -7.275	0.50	37.19
	ATOM	122	С	BASP	Α	321	29.123	-2.565 -7.253	0.50	36.68
	ATOM	123	0	AASP	Α	321	28.820	-2.861 -8.434	0.50	36.87
	ATOM	124	0	BASP	A	321	28.934	-2.942 -8.411	0.50	
	MOTA	125	N	ΑĻΑ	A	322	28.374	-2.968 -6.235	1.00	36.08
30	MOTA	126	CA	ALA	À	322	27.268	-3.902 -6.417		35.35
	ATOM	127	CB	ALA	A	322	27.124	-4.781 -5.175	1.00	31.59
	ATOM	128	C	ALA_	A	322	25.946		1.00	30.73
	ATOM	129	ō	ALA	A	322		-3.204 -6.709	1.00	30.07
	ATOM	130	N	GĻŲ	À	323	24.955	-3.857 -7.036	1.00	26.53
35	ATOM	131	CA	GLU:	A		25.932	-1.880 -6.596	1.00	27.98
	ATOM	132	CB	GLU		323	24.713	-1.117 -6.827	1.00	29.88
	ATOM	133	CG	GLU	A	323	25.027	0.380 -6.855	1.00	30.98
	ATOM	134	CD	GĽÚ.	A	323	24.870	1.068 -5.509	1.00	31.62
	ATOM	135	OE1		A	323	23.463	0.940 -4.960	1.00	31.98
40	ATOM	136		GLU	A	323	23.183	-0.056 -4.257	1.00	33.10
.0	ATOM	137	OE2	GĽŬ.	A	323	22.640	1.836 -5.233	1.00	30.01
	ATOM		C	GLU	A	323	24.010	-1.515 -8.123	1.00	30.86
	ATOM	138	0	GLŲ.	A	323	24.655	-1.705 -9.151	1.00	28.86
		139	N	PRO	A	324	22.674	-1.659 -8.083	1.00	30.66
45	ATOM	140	CD	PRO	A	324	21. 7 74	-1.466 -6.935	1.00	31.01
43	ATOM	141	CA	PRO	A	324	21.935	-2.032 -9.290	1.00	30.29
	ATOM	142	CB	PRO	Α	324	20.613	-2.598 -8.760	1.00	31.42
	ATOM	143	CG	PRO	A	324	20.626	-2.363 -7.258	1.00	33.66
	MOTA	144	С	PRO	A	324	21.717	-0.785-10.138	1.00	27.46
	ATOM	145	0	PŖĢ	Α	324	21.893	0.332 -9.668	1.00	26.19
50	ATOM	146	N	PRO	Α	325	21.335	-0.959-11.403	1.00	27.80
	ATOM	147	CD	PRO	Α	325	21.082	-2.198-12.161	1.00	27.35
	ATOM	148	CA	PRO	Α	325	21.125	0.242-12.211	1.00	25.59
	MOTA	149	CB	PRO	Α	325	21.258	-0.266-13.637	1.00	
	ATOM	150	CG	PRO	Ä	325	20.773	-1.695-13.559		24.02
55	ATOM	151	C	PRO	Α	325	19.749	0.830-11.954	1.00	26.00
	ATOM	152	ō	PRO	A	325			1.00	23.73
	ATOM	153	N	ILE	A	325	18.873	0.165-11.402	1.00	24.83
	ATOM	154	CA	ILE	A		19.571	2.081-12.352	1.00	22.11
	ATOM	155	CB	ILE	A	32 <i>6</i>	18.296	2.762-12.212	1.00	24.01
60	ATOM	156	CG2	ILE	A	326	18.502	4.282-12.133	1.00	25.97
	ATOM	157	CG2	ILE		326	17.168	4.992-12.286	1.00	20.75
		±J/	CGI	THE	A	326	19.189	4.632-10.805	1.00	29.31

								6.120-10.525	1.00 3	2.91
5	MOTA	158	CD1	ILE .		326	19.301	2.408-13.471		5.72
	ATOM	159	С	ILE .	A	326	17.506			5.55
	ATOM	160	0	ILE	A	326	17.906	2.758-14.581		5.57
	ATOM	161	N	LEU	A	327	16.392	1.703-13.301		3.80
		162	CA		Α	327	15.595	1.279-14.439		
10	MOTA	163	CB		A	327	14.872	-0.029-14.104	_	23.96
10	ATOM		CG	LEU	A	327	15.778	-1.210-13.728		19.89
	MOTA	164		LEU	Α	327	14.944	-2.462-13.583		21.19
	MOTA	165	CD1		A	327	16.850	-1.415-14.805		17.53
	ATOM	166	CD2	LEU		327	14.598	2.317-14.935	1.00	27.16
	MOTA	167	C	LEU	A		14.161	3.202-14.194	1.00	25.98
15	MOTA	168	0	LEU	A	327	14.251	2.207-16.210	1.00	26.56
	MOTA	169	N	TYR	Α	328	13.303	3.123-16.814	1.00	24.45
	MOTA	170	CA	TYR	A	328		3.465-18.245	1.00	26.72
	MOTA	171	CB	TYR	Α	328	13.724	4.693-18.314		27.73
	MOTA	172	CG	TYR	A	328	14.587	5.949-18.518		28.56
20	ATOM	173	CD1	TYR	A	328	14.021			29.10
	MOTA	174	CE1	TYR	Α	328	14.798	7.092-18.509		26.01
	ATOM	175	CD2	TYR	Α	328	15.962	4.612-18.110		30.63
	MOTA	176	CE2	TYR	A	328	16.750	5.753-18.098	1.00	
	ATOM	177	CZ	TYR	Α	328	16.157	6.988-18.297	1.00	30.07
25		178	OH	TYR	Α	328	16.917	8.130-18.265	1.00	37.94
25	ATOM	179	C	TYR	A	328	11.923	2.501-16.827	1.00	24.95
	ATOM		0	TYR	A	328	11.774	1.274-16.846	1.00	27.02
	MOTA	180		SER	A	329	10.912	3.358-16.800	1.00	25.60
	MOTA	181	N	SER	Ā	329	9.533	2.908-16.837	1.00	29.45
	MOTA	182	CA			329	8.661	3.858-16.020	1.00	30.80
30	MOTA	183	CB	SER	A	329	7.297	3.721-16.364		33.74
	MOTA	184	OG	SER	A		9.129	2.947-18.313		31.30
	MOTA	185	С	SER	A	329	9.908	3.397-19.154		27.35
	MOTA	186		SER	A	329	7.930	2.469-18.629		32.98
	MOTA	187		GĽÚ	Α	330		2.482-20.00		35.10
35	MOTA	188		GĽÜ	A	330	7.459	1.968-20.074		34.67
	MOTA	189	CB	GLÜ	A	330	6.031	3.924-20.50		40.06
	MOTA	190	C	GĻŪ	A	330	7.532	4.841-19.82		42.65
	MOTA	191	. 0	GĽŪ	Α	330	7.068	4.126-21.68		41.16
	MOTA	192	N	TYR	Α	331	8.124	5.470-22.23		42.66
40		193	CA	TYR	Α	331	8.263		_	42.54
,,,	ATOM	194	CB	TYR	Α	331	9.323	5.482-23.35		38.67
	MOTA	195		TYR	A	331	9.202	4.347-24.34		34.66
	ATOM	196		TYR	Α	331	10.105	3.284-24.33		34.89
	MOTA	19			Α	331	9.985	2.228-25.23	3 1.00	37.88
45		198			A	331	8.174		7 1.00	34.65
43	MOTA	19				331	8.045	3.276-26.19	3 1.00	
		20		TYR			8.950	2.232-26.15	9 1.00	
	MOTA	20		TYR			8.814	1.191-27.04		
	MOTA			TYR			6.943	6.043-22.75		
	MOTA	20:		TYR			6.018		6 1.00	
50		20					6.868		2 1.00	
	MOTA	20		ASF			5.684			52.40
	MOTA	20		ASF			5.781		72 1.00	52.86
	MOTA	20		ASI			4.356			
	MOTA	20		ASI						
5:		20	8 0	ASI			3.561		_	
	MOTA	20	9 N	PRO) A		4.103			_
	ATOM	21		PRO) A		4.962		53 1.00	
	MOTA	21			O P		2.84			_
	ATOM					333	3.07			_
4	MOTA 0					333				
O	MOTA U			PR		A 333		3 7.478-21.3	98 1.00	J 36.1/
	AIOM	2.		- • •	_					

5	ATOM	215	. 0	PRO		222				
	ATOM	216	-	THR		333	1.879		5 1.00	
	ATOM	217		THR		334	0.457			52.26
	ATOM	218		THR		334	-0.724			54.21
	ATOM	219				334	-1.997			53.90
10	ATOM	220		THR		334	-1.971			53.92
	ATOM	221				334	-3.237			
	ATOM			THR		334	-0.864		1.00	
	ATOM	222		THR		334	-1.389	8.443-19.46	1.00	
	ATOM	223		ARG		335	-0.386	10.002-20.76	1.00	
15	ATOM	224		ARG	A	335	-0.377			
13		225		ARG	Α	335	-0.569			
	ATOM	226		ARG	Α	335	-1.349		7 1.00	
	ATOM	227		ARG	Α	335	-0.919	10.908-17.479		
	ATOM	228	N	PRO	Α	336	-2.667	11.015-18.889	1.00	
20	ATOM	229	CD	PRO	A	336	-3.389	11.117-20.165	1.00	
20	MOTA	230	CA	PRO	A	336	-3.587	10.915-17.752	1.00	
	ATOM	231	CB	PRO	A	336	-4.911	11.456-18.302		
	ATOM	232	CG	PRO	Α	336	-4.645	11.809-19.760		
	ATOM	233	C	PRO	Ą	336	÷3.698	9.468-17.279		51.33
	MOTA	234	0	PRO	A	336	-4.340	8.644-17.929		49.25
25	MOTA	235	N	PHE	A	337	-3.063	9 170 16 749		48.06
	MOTA	236	CA	PHE	А	337	-3.055	9.170-16.147		47.90
	ATOM	237	CB	PHE	A	337	-2.063	7.821-15.582		46.61
	MOTA	238	CG	PHE	Α	337	-0.649	7.732-14.421		47.73
	ATOM	239	CD1	PHE	A	337	-0.017	8.011-14.805		46.27
30	ATOM	240	CD2	PHE	A	337		9.168-14.368		46.55
	ATOM	241	CE1	PHE	A	337	0.061	7.113-15.591		48.12
	ATOM	242	CE2	PHE	A	337	1.305	9.429-14.707		48.09
	ATOM	243	CZ	PĤĘ	A	337	1.386	7.364-15.938		47.57
	ATOM	244	C	PHE	A	337	2.009	8.525-15.495	1.00	48.40
35	ATOM	245	ō	PHE	A	337	-4.401	7.338-15.071	1.00	46.15
	ATOM	246	N	SER	A		-5.250	8.127-14.671	1.00	48.34
	ATOM	247	CA	SER		338	-4.573	6.022-15.080	1.00	45.06
	ATOM	248	CB	SER	A A	338	-5.781	5.385-14.578	1.00	45.12
	ATOM	249	OG	SER		338	-6.477	4.594-15.684	1.00	44.49
40	ATOM	250	C	SER	Ā	338	-6.227	3.206-15.554	1.00	45.78
	ATOM	251	0	SER	A	338	-5.292	4.439-13.488	1.00	47.04
	ATOM	252	N		A	338	-4.090	4.186-13.387	1.00	44.08
	ATOM	253	CA	GĽÚ	À	339	-6.206	3.916-12.676	1.00	45.63
	ATOM	254	CB	GLU	A	339	-5.802	3.012-11.608	1.00	45.40
45	ATOM	255	CG	GĻÜ	A	339	-7.015	2.521-10.814	1.00	45.66
	ATOM	256		GLU	A	339	-6.637	1.680 -9.600	1.00	46.81
	ATOM	257	CD	GLU	A	339	-7.717	1.652 -8.535	1.00	47.56
	ATOM	258	OE1	GĻŲ	A	339	-8.471	0.656 -8.477	1.00	47.37
	ATOM		OE2	GĽÚ	Α	339	-7.810	2.625 -7.754	1.00	49.29
50	ATOM	259	C	GĽÚ	A	339	-5.040	1.821-12.170	1.00	45.23
50	ATOM	260	0	GLU	A	339	-3.862	1.641-11.872	1.00	46.51
		261	N	ALA	Α	340	-5.712	1.010-12.982	1.00	42.87
	ATOM	262	CA	АĻА	Α	340	-5.078	-0.158-13.574	1.00	40.24
	ATOM	263	CB	ALA	A	340	-6.055	-0.871-14.496	1.00	41.40
55	ATOM	264	C	ALA	A	340	-3.837	0.273-14.350	1.00	38.83
55	ATOM	265	0	ALA	Α	340	-2.909	-0.515-14.543		
	ATOM	266	N	SER	Α	341	-3.836	1.535-14.543	1.00	35.58
	ATOM	267	CA	SER	A	341	-2.742		1.00	35.79
	ATOM	268	CB	SER	A	341	-3.231	2.133-15.537	1.00	36.58
	ATOM	269	OG	SER	A	341	-2.211	3.454-16.154	1.00	39.01
60	ATOM	270	C	SER	A	341		4.130-16.864	1.00	36.09
	ATOM	271	0	SER	A	341	-1.480	2.376-14.691	1.00	35.63
						~ 4 1	-0.389	1.913-15.038	1.00	33.20

_	» mon	272	N	MET A	. 3	42	-1.626	3.115-13.595 1.00 35.92
	ATOM	273		MET A		42	-0.498	3.396-12.708 1.00 35.88 4.396-11.623 1.00 35.96
	MOTA	274		MET A	_	342	-0.912	4.550 == 0
	ATOM	275		MET A		342	0.241	5.218-11.059 1.00 38.02
	MOTA	276		MET A	_	342	-0.308	6.374 -9.780 1.00 44.73
••	MOTA	277				342	0.626	7.815-10.205 1.00 42.49
10	MOTA		C			342	-0.011	2.100-12.059 1.00 34.17
	MOTA	278	0			342	1.195	1.880-11.909 1.00 33.40
	MOTA	279	Ŋ	•		343	-0.957	1.243-11.687 1.00 29.95
	MOTA	280				343	-0.640	-0.034-11.062 1.00 31.96
_	MOTA	281	CA		A	343	-1.921	-0.810-10.751 1.00 31.70
15	MOTA	282	CB		A	343	-2.667	-0.337 -9.502 1.00 37.13
	MOTA	283	CG		A	343	-1.749	-0.507 -7.940 1.00 36.00
	MOTA	284	SD		A	343	-1.468	-2.299 -7.886 1.00 32.14
	ATOM	285	CE		A	343	0.234	-0.875-11.979 1.00 31.72
	MOTA	286	С		A	343	1.159	-1.558-11.527 1.00 30.26
20	MOTA	287	0	MET	A	344	-0.069	-0.823-13.272 1.00 29.04
	MOTA	288	N	GLY		344	0.688	-1.591-14.242 1.00 24.94
	MOTA	289	CA	GLY	A	344	2.104	-1.085-14.396 1.00 26.01
	MOTA	290	C	GLY	A	344	3.046	-1.873-14.463 1.00 28.72
	MOTA	291	0	GLY	A	345	2.257	0.232-14.471 1.00 26.97
25	ATOM	292	N	LEU	A	345	3.576	0.839-14.608 1.00 31.15
	MOTA	293	CA	LEU	A	345	3.459	2.361-14.753 1.00 30.06
	MOTA	294	CB	LEU	A	345 345	2.765	2.924-15.995 1.00 33.50
	MOTA	295	CG	LEU	A	345 345	2.901	4.439-15.999 1.00 33.52
	MOTA	296	CD1	LEÜ	A		3.379	2 324-17.257 1.00 33.22
30	MOTA	297	CD2	LEU	À	345	4.433	0.534-13.383 1.00 30.31
	MOTA	298	C	rén	A	345	5.564	0.061-13.505 1.00 32.80
	MOTA	299	0	LEÜ	A	345	3.884	0.813-12.205 1.00 27.83
	MOTA	300	N	LEU	A	346	4.595	0 596-10.947 1.00 26.19
	MOTA	301		LEU	A	346	3.729	1.063 -9.783 1.00 24.51
35	MOTA	302		ΓËΩ	A	346	3.483	2.569 -9.682 1.00 26.33
	MOTA	303		LEU	A	346	2.623	
	MOTA	304		ΓĔÜ	Ä	346	4.809	2 527 3 00 24 89
	MOTA	305		LEU	A	346	5.032	707 1 00 25 72
	MOTA	306		LEU	Α	346	6.181	00 00 06
40	MOTA	307	0	LEU	Α	346	4.117	007 1 00 23 90
	MOTA	308		THR	Α	347	4.117	
	MOTA	309		THR	A	347		1 00 26 39
	MOTA	310		THR	A	347	3.164	24 24 24 24 27
	MOTA	31:			A	347	2.421	1 00 23 98
45	MOTA	31:	2 CG2		A	347	2.301	1 00 06 17
	MOTA	31	3 C	THR	Ą	347	5.366	1 00 27 44
	ATOM	31	4 0	THR	A	347	6.176	
	MOTA	31	5 N	ASN	A	348	5.242	2 -3.13. 1 000 1 00 23 77
	MOTA	31	6 CA	aşn	Α	348	6.092	2 -3.017 117000
50		31	7 CB	asn	Α	348	5.65	7 22.520 15.500
	MOTA	31	8 CG	aşņ	A	348	6.52	2 3.302 25151 1 00 24 81
	ATOM	31	9 OD:	1 ASN	A	348	7.61	6 -2.755 ±0.110 32 61
	MOTA	32		2 ASN	Α	348	6.01	0 24.250 1.150
	ATOM			ASN	Α	348	7.53	2 = 3.225 13.722 =
5	5 ATOM			ASN	Α		8.45	3 -4.027 13.070 -
,	ATOM			LEU	I A	349	7.71	1 -1.555 15-1
	ATOM					349	9.03	
	ATOM					349	8.92	.9 -0.020 1 00 22 64
	ATOM		26 CG			349	10.15	0.075 == 0.07 1 00 10 35
4	MOTA 06		27 CE			349	11.22	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
•	MOTA		28 CI			349	9.72	26 2.040-11.415 1.00 21.97
	AION				•			

5	ATOM	329	С	LEU	А	349	9.564	-2 225 11 524	1 00	
	ATOM	330	ō	LEU	A	349	10.724	-2.335-11.734 -2.749-11.717		22.94
	ATOM	331	N	ALA	A	350	8.705	-2.749-11.717	1.00	23.97
	ATOM	332	CA	ALA	A	350	9.113		1.00	21.67
	ATOM	333	CB	ALA	A	350		-3.356 -9.586	1.00	21.83
10	ATOM	334	c	ALA	A	350	7.963	-3.441 -8.593	1.00	18.95
	ATOM	335	Ö	ALA	A	350	9.568	-4.757 -9.985	1.00	21.90
	ATOM	336	N	ASP			10.625	-5.221 -9.554	1.00	24.15
	ATOM	337	CA	ASP	A A	351	8.767	-5.423-10.810	1.00	23.24
	ATOM	338	CB	ASP		351	9.093	-6.772-11.259	1.00	25.87
15	ATOM	339	CG		A	351	8.028	-7.274-12.239	1.00	27.03
	ATOM	340	OD1	ASP	A	351	8.103	-8.772-12.458	1.00	31.64
	ATOM	341	OD2	ASP	A	351	8.217	-9.196-13.628	1.00	35.06
	ATOM	342		ASP	A	351	8.049	-9.525-11.464	1.00	36.86
	ATOM	343	C	ASP	A	351	10.469	-6.825-11.912	1.00	22.36
20	ATOM		0	ASP	A	351	11.219	-7.773-11.702	1.00	25.15
20	ATOM	344	N	ARG	A	352	10.810	-5.808-12.697	1.00	23.58
	ATOM	345	CA	ARG	A	352	12.115	-5.787-13.347	1.00	21.07
	ATOM	346	CB	ARG	A	352	12.120	-4.785-14.507	1.00	21.02
	ATOM	347	CG	ARG	Α	352	11.539	-5.352-15.797	1.00	20.44
25		348	CD	ARG	A	352	11.554	-4.319-16.915	1.00	20.43
2,5	ATOM ATOM	349	NE	ARG	Α	352	10.592	-3.245-16.687	1.00	19.85
	ATOM	350	CZ	ARG	Α	352	10.910	-1.954-16.641	1.00	19.69
		351	NH1	ARĞ	A	352	12.172	-1.564-16.813	1.00	17.36
	ATOM	352	NH2	ARG	A	352	9.962	-1.049-16.441	1.00	21.88
30	ATOM	353	C	AŖĢ	A	352	13.223	-5.442-12.350	1.00	22.11
30	ATOM	354	0	ARG	A	352	14.346	-5.945-12.454	1.00	24.13
	ATOM	355	N	GLU	A	353	12.909	-4.587-11.383	1.00	18.66
	ATOM ATOM	356	CA	GLÜ	A	353	13.888	-4.206-10.376	1.00	19.08
		357	CB	GĻU	Α	353	13.317	-3.102 -9.483	1.00	21.62
35	ATOM ATOM	358	CG	GĽÜ	A	353	13.295	-1.718-10.114	1.00	20.97
33	ATOM	359	CD	GĽŪ	Ą	353	12.832	-0.648 -9.129	1.00	23.84
	ATOM	360	OE1	GĻŪ	A	353	11.611	-0.531 -8.926	1.00	24.76
		361	OE2	GĻŲ	Α	353	13.686	0.066 -8.557	1.00	24.95
	ATOM ATOM	362	C	GLÜ	A	353	14.246	-5.423 -9.512	1.00	20.14
40		363	0	GLU	A	353	15.398	-5.600 -9.104	1.00	19.40
70	ATOM ATOM	364	N	ΓΕŬ	A	354	13.246	-6.257 -9.235	1.00	19.54
		365	CA	ΓĔΩ	Α	354	13.434	-7.452 -8.415	1.00	21.77
	ATOM	366	CB	LEU	A	354	12.107	-8.209 -8.270	1.00	23.09
	ATOM ATOM	367	CG	LEU	A	354	11.160	-7.606 -7.223	1.00	25.00
45	ATOM	368	CD1	LEU	A	354	9.720	-8.013 -7.510	1.00	23.49
45	ATOM	369	CD2	ΓËΩ	A	354	11.584	-8.069 -5.839	1.00	23.31
		370	C	LEU	Α	354	14.500	-8.386 -8.981	1.00	23.21
	ATOM	371	0	LEU	Α	354	15.255	-9.007 -8.234	1.00	22.44
	ATOM	372	N	VAL	Α	355	14.560	-8.490-10.302	1.00	22.52
50	ATOM	373	CA	VAL	Α	355	15.551	-9.343-10.935	1.00	21.66
30	ATOM	374	CB	VAJ.	A	355	15.353	-9.365-12.466	1.00	24.35
	ATOM	375	CG1	ΛÝŢ	Α	355	16.435	-10.214-13.119	1.00	28.16
	ATOM	376	CG2	VAL	A	355	13.957	-9.886-12.798	1.00	21.59
	ATOM	377	С	VAL	A	355	16.944	-8.811-10.606	1.00	23.74
55	ATOM	378	0	VAL	Α	355	17.857	-9.581-10.291	1.00	23.51
55	ATOM	379	N	HIS	A	356	17.105	-7.489-10.669	1.00	21.27
	ATOM	380	CA	HIS	Α	356	18.392	-6.861-10.369	1.00	21.31
	ATOM	381	CB	HIS	Α	356	18.384	-5.390-10.811	1.00	19.87
	ATOM	382	CG	HIS	Α	356	18.494	-5.205-12.295	1.00	21.77
60	ATOM	383	CD2	HIS	A	356	17.543	-5.048-13.248	1.00	21.66
60	ATOM	384	ND1	HIS	A	356	19.704	-5.177-12.955	1.00	21.11
	ATOM	385	CE1	HIS	Α	356	19.496	-5.011-14.249	1.00	24.96

							18.192 -4.931-14.455 1.00 18.37
5 '	MOTA	386	NE2	HIS	Α	356	18.192
-	MOTA	387	С	HIS	Α	356	10.702
	ATOM	388	0	HIS	A	356	19.004
	ATOM	389	N	MET	Α	357	17.800
	ATOM	390	CA	MET	Α	357	17.037
10	ATOM	391	СВ	MET	Α	357	18.303
10	ATOM	392	CG	MET	Α	357	10.025 0.575 1.00 23 64
	MOTA	393	SD	MET	Α	357	15.051
	MOTA	394	CE	MET	Α	357	14.189 -5.332 -4.163 1.00 23.13
	MOTA	395	C	MET	Α	357	18.411 -8.259 -6.192 1.00 23.69
15		396	Ö	MET	A	357	19.337 -8.328 -5.389 1.00 24.41
13	MOTA	397	N	ILE	Α	358	17.856 -9.331 -6.746 1.00 27.14
	MOTA	398	CA	ILE	A	358	18.314 -10.672 -6.425 1.00 28.79
	ATOM		CB	ILE	A	358	17.529 -11.725 -7.232 1.00 32.42
	MOTA	399	CG2	ILE	A	358	18.267 -13.064 -7.220 1.00 32.77
	MOTA	400	CG2	ILE	Α	358	16.125 -11.880 -6.644 1.00 31.94
20	MOTA	401	CD1	ILE	A	358	15.062 -12.196 -7.680 1.00 34.85
	MOTA	402	CDI	ILE .	A	358	19.801 -10.802 -6.728 1.00 28.75
	MOTA	403		ILE	A	358	20.569 -11.305 -5.912 1.00 31.60
	MOTA	404	0	ASN	A	359	20.207 -10.325 -7.897 1.00 27.91
	MOTA	405	N	ASN	A	359	21,601 -10.401 -8.293 1.00 29.16
25	MOTA	406	CA	ASN	Ā	359	21.721 -10.172 -9.801 1.00 31.88
	MOTA	407	CB	ASN	A	359	21.253 -11.381-10.599 1.00 39.34
	ATOM	408	CG	ASN	A	359	21.916 -12.422-10.612 1.00 41.27
	MOTA	409	OD1		Ā	359	20.102 -11.255-11.253 1.00 38.58
	MOTA	410	ND2	ASN	Ą	359	22.476 -9.436 -7.510 1.00 30.75
30	MOTA	411	C	ASN	A	359	23.686 -9.629 -7.412 1.00 33.35
	MOTA	412	. 0	ASN	A	360	21.872 -8.400 -6.940 1.00 30.07
	MOTA	413	N	TRP	A	360	22.634 -7.451 -6.132 1.00 27.87
	ATOM	414	CA	TRP	A	360	21.849 -6.150 -5.948 1.00 24.80
	MOTA	415	CB	TRP		360	22 196 -5.392 -4.691 1.00 23.04
35	MOTA	416	CG	TRP	A À	360	21.501 -5.443 -3.438 1.00 19.83
	MOTA	417	_	TRP	A	360	22 147 -4.543 -2.564 1.00 22.31
	MOTA	418		TRP	À	360	20 392 -6.165 -2.972 1.00 20.09
	MOTA	419		TRP	A N	360	23.212 -4.488 -4.529 1.00 18.99
	ATOM	420		TRP	À	360	23.187 -3.974 -3.255 1.00 21.17
40		421			A		21 721 -4.340 -1.243 1.00 20.43
	MOTA	422					19 968 -5.965 -1.661 1.00 20.12
	MOTA	423					20.635 -5.057 -0.812 1.00 18.54
	MOTA	424		ئد بند	_		22 892 -8.099 -4.766 1.00 24.88
	MOTA	425		TRE			23.978 -7.980 -4.198 1.00 25.00
45		426		TŘĘ			21 879 -8.789 -4.252 1.00 24.08
	MOTA	42		ALA			21.972 -9.462 -2.958 1.00 26.06
	MOTA	428		ALA			20.676 -10.203 -2.672 1.00 20.27
	MOTA	42		AĻĄ			23.161 -10.433 -2.897 1.00 28.44
	MOTA	43		ALA			23.843 -10.531 -1.876 1.00 28.95
50	MOTA (43		AĮ.i			23.414 -11.144 -3.992 1.00 31.41
	MOTA	43		LYS			24.530 -12.097 -4.047 1.00 33.33
	MOTA	43					24.564 -12.824 -5.390 1.00 34.81
	MOTA	43	4 CB				24.304 12.604 1 00 36 27
	ATOM	43					23.319 -13.608 -5.756 1.00 36.27 23.458 -14.178 -7.167 1.00 38.30
5	5 ATOM	43	6 CD			A 362	23.456 -14.170 -1
	ATOM	43	7 CE			A 362	22.363 -13.133 /
	ATOM	43	8 NZ			A 362	22.111 -13.322
	ATOM	43	9 C	LY		A 362	25.054 -11.551
	ATOM			LY	*	A 362	20.860 -11.577 - 5.50 - 24 23
6	O ATOM		1 N		•	A 363	25.826 -10.033 -10.03
·	ATOM			BA	ŖĠ	A 363	25.826 -10.059 -4.095 0.50 34.03
	3.22.344						

	•										
5	ATOM	443	CA	AARG	A	363	27.035	-9.254	-3.987	0.50	33.25
	ATOM	444	CA	BARG	A	363	27.035	-9.254	-3.987	0.50	32.83
	ATOM	445	CB	AARG	Α	363	27.031		-5.044	0.50	34.67
	ATOM	446	CB	BARG	Α	363	27.031		-5.045	0.50	34.20
	ATOM	447	CG	AARG	Α	363	26.933		-6.478	0.50	36.32
10	ATOM	448	CG	BARG	Α	363	26.930		-6.480	0.50	35.56
	ATOM	449	CD	AARG	A	363	27.745		-7.415	0.50	38.39
	MOTA	450	CD	BARG	A	363	27.752		-7.414	0.50	37.18
	ATOM	451	NE	AARG		363	29.171		-7.091	0.50	39.98
	ATOM	452	NE		Α	363	27.195		-8.762	0.50	37.39
15	ATOM	453	CZ		A	363	30.086		-7.692	0.50	40.54
	ATOM	454	CZ		A	363	27.905		-9.855	0.50	
	ATOM	455	NH1	AARG	A	363	29.735		-8.675		40.02
	ATOM	456	NH1	BARG	A	363				0.50	38.13
	ATOM	457	NH2	AARG	A	363	29.205		-9.761	0.50	40.42
20	ATOM	458	NH2	BARG			31.358		-7.326	0.50	43.19
20	ATOM	459	C			363	27.311		-11.041	0.50	38.91
	ATOM	460	C		A	363	27.207		-2.610	0.50	33.28
				BARG		363	27.207		-2.610	0.50	32.81
	ATOM	461	0		A	363	28.223		-2.344	0.50	34.18
25	ATOM	462	0	BÂRG	A	363	28.223		-2.345	0.50	33.43
23	ATOM	463	N	VAL	A	364	26.215		-1.740	1.00	33.12
	ATOM	464	CA	VAL	A	364	26.288		-0.389	1.00	33.63
	ATOM	465	CB	VAL	Α	364	24.898	-8.178	0.292	1.00	34.97
	ATOM	466	CG1	VAL	Α	364	25.036	-7.608	1.700	1.00	35.44
20	ATOM .	467	CG2	VAL	A	364	23.946		-0.532	1.00	36.69
30	ATOM	468	C	VAL	A	364	27.184	-9.157	0.428	1,.00	34.27
	ATOM	469	0	VAL	A	364	26.878	-10.341	0.603	1.00	34.95
	ATOM	470	N	PRO	A	365	28.306	-8.626	0.935	1.00	36.08
	ATOM	471	CD	PRO	A	365	28.775	-7.235	0.793	1.00	34.84
25	ATOM	472	CA	PRO .	A	365	29.231	-9.442	1.733	1.00	37.82
35	ATOM	473	CB	PRO	Α	365	30.110	-8.408	2.430	1.00	34.31
	ATOM	474	CG	PRO	Α	365	30.127	-7.247	1.475	1.00	37.77
	ATOM	475	С	PRO	Α	365	28.538	-10.373	2.720	1.00	37.61
	ATOM	476	0	PRO	Α	365	27.692	-9.945	3.507	1.00	37.74
40	ATOM	477	N	$\operatorname{\mathbf{GLY}}$	A	366	28.890	-11.654	2.654	1.00	39.04
40	ATOM	478	CA	GLY	Α	366	28.307	-12.635	3.554	1.00	38.27
	MOTA	479	С	GĽŸ	Α	366	26.991	-13.264	3.138	1.00	39.32
	MOTA	480	0	GLY	Α	366	26.638	-14.336	3.635	1.00	39.53
	ATOM	481	N	PHE	Α	367	26.246	-12.615	2.236	1.00	38.60
	MOTA	482	CA	PHE	Α	367	24.960	-13.148	1.783	1.00	36.36
45	ATOM	483	CB	PHE	Α	367	24.281	-12.178	0.808	1.00	32.10
	ATOM	484	CG	PHE	Α	367	22.827	-12.473	0.581	1.00	30.12
	ATOM	485	CD1	PHE	Ά	367	22.401	-13.083	-0.596	1.00	28.95
	ATOM	486	CD2	PHE	Α	367		-12.176	1.563	1.00	26.18
	ATOM	487	CE1	PHE	Α	367		-13.400		1.00	29.42
50	ATOM	488	CE2	PHE	A	367		-12.491	1.373	1.00	27.60
	ATOM	489	CZ	PHE	Α	367		-13.103	0.196	1.00	26.81
	ATOM	490	С	PHE	Α	367	25.072	-14.519	1.117	1.00	36.82
	ATOM	491	0	PHE	Α	367		-15.398	1.359	1.00	36.55
	ATOM	492	N	VAL	Α	368		-14.694	0.276	1.00	38.28
55	ATOM	493	CA	VAL	A	368		-15.965			
	ATOM	494	CB	VAL	A	368		-15.850		1.00	42.34
	ATOM	495	CG1	VAL	A	368		-13.830		1.00	41.78
	ATOM	496	CG2	VAL	A	368				1.00	44.60
	ATOM	497	CG2	VAL	A	368		-15.457		1.00	42.23
60	ATOM	498	0	VAL	A			-17.100	0.533	1.00	43.85
	ATOM	499	N	ASP		368	26.469	-18.274	0.216	1.00	44.85
		マフフ	₹A	H2 P	Α	369	27.199	-16.750	1.699	1.00	44.93

_			C3	ASP A	Ą	369	27.579 -17.755 2.688 1.00 44.96 °
5	ATOM	500				369	28.336 -17.106 3.849 1.00 43.76
	ATOM	501				369	29.608 -16.413 3.404 1.00 43.04
	ATOM	502			A	369	30.121 -15.570 4.167 1.00 44.32
	MOTA	503			A	369	30.097 -16.709 2.293 1.00 46.76
	ATOM	504			A	369	26 340 -18.465 3.228 1.00 45.89
10	ATOM	505	C		A	369	26.360 -19.671 3.475 1.00 48.61
	MOTA	506	0		A	370	25.261 -17.714 3.407 1.00 43.59
	ATOM	507	N		A	370	24 020 -18.279 3.924 1.00 44.24
	MOTA	508	CA		A	370	22 980 -17.173 4.110 1.00 41.42
_	MOTA	509	CB		A	370	23 404 -16.015 5.014 1.00 41.45
15	MOTA	510	CG		A	370	22 219 -15.095 5.245 1.00 42.25
	MOTA	511	CD1	LEU	A	370	23 931 -16.552 6.332 1.00 38.35
	MOTA	512	CD2	LEU		370	23.449 -19.360 3.013 1.00 44.03
	MOTA	513	C	LEU	A	370	23.773 -19.423 1.829 1.00 43.63
	MOTA	514	0	LEU	A	371	22.593 -20.206 3.575 1.00 44.29
20	ATOM	515	N	THR	A	371	21 968 -21.272 2.806 1.00 44.84
	MOTA	516	CA	THR	A	371	21.293 -22.302 3.730 1.00 45.65
	MOTA	517	CB	THR	A		20.262 -21.663 4.495 1.00 46.43
	MOTA	518	OG1	THR	A	371	22.314 -22.903 4.677 1.00 46.48
	MOTA	519	CG2	THR	A	371 371	20.923 -20.684 1.864 1.00 44.93
25	ATOM	520	С	THR	A		20.418 -19.585 2.092 1.00 44.36
	MOTA	521	0	THR	A	371	20.607 -21.418 0.804 1.00 43.83
	MOTA	522	N	LEU	A	372	19.624 -20.971 -0.166 1.00 44.62
	MOTA	523	CA	LEU	A	372	19.407 -22.043 -1.237 1.00 47.17
	MOTA	524	CB	LEU	A	372	18.512 -21.690 -2.429 1.00 46.91
30	MOTA	525	CG	ΓÉΩ	A	372	19.005 -20.417 -3.098 1.00 48.73
	MOTA	526	CD1	LEU	A	372	18.521 -22.844 -3.420 1.00 51.12
	ATOM	527	CD2	LEU	A	372	18.307 -20.644 0.512 1.00 44.84
	MOTA	528	С	rën	À	372	17.705 -19.602 0.261 1.00 43.25
	MOTA	529	0	TEÑ	À	372	17.849 -21.558 1.382 1.00 43.14
35	MOTA	530	N	HIŞ	A	373	16.599 -21.353 2.100 1.00 42.23
	MOTA	531	CA	HIS	A	373	16.318 -22.525 3.062 1.00 45.38
	MOTA	532	CB	HIS	A	373	15.114 -22.315 3.934 1.00 51.43
	MOTA	533	CG	HIS	A	373	13.808 -22.621 3.743 1.00 54.99
	MOTA	534		HIS	A	373	15.187 -21.716 5.174 1.00 54.26
40	MOTA	535		HIS	A	373	13.979 -21.663 5.709 1.00 53.77
	MOTA	536		HIS	A	373	13.124 -22.206 4.861 1.00 55.27
	MOTA	537		HIS	A	373	16.665 -20.047 2.885 1.00 39.78
	MOTA	538		HIS	A	373	15.677 -19.324 2.971 1.00 37.71
	MOTA	539		HIS	A	373	17.839 -19.738 3.440 1.00 36.38
45	ATOM	540		ASP	A	374	18.020 -18.516 4.219 1.00 37.21
	MOTA	541		ASP	A		10.020 10.020 1 00 39 17
	MOTA	542		ASP	A		19.287 -18.620 5.073 1.00 33.17 19.064 -19.425 6.344 1.00 41.47
	MOTA	543		ASP	A		19.004 13.110 1 00 37 09
	ATOM	544			À		17.896 -19.543 6.772 1.00 37.05 20.052 -19.940 6.912 1.00 44.40
50	MOTA	545	5 OD2		Α		20.032
	ATOM	546	6 C	ASP	A		18.083
	MOTA	541	7 0	AŞP			17.396 10.200
	MOTA	54	8 N	GĻN	A		10.000 -17.334
	MOTA	54	9 CA	GLN			18.700 -10.555 -1.255 - 20. 20. 21
55		55	o CB	GLN			19.634 -10.756 6.666
	MOTA	55	1 CG	GLN			21.125
	ATOM	55		GLN	P		21.920 -17.222 - 0.00 36 09
	ATOM			L GLN	P		21.4/6 -17.20, 200 1 00 40 32
	MOTA			2 GLN	į P	375	23.097 -17.730 0.00-
6				GLN		375	17.379 10.000
3	ATOM			GLN		375	16.990 -14.840 0.653 1.00 27.42

5	ATOM	557	N	VAL	A	376	16.617	-17.056	0.429	1.00	30.38
	ATOM	558	CA	VAL	A	376	15.242	-16.907		1.00	33.50
	ATOM	559	CB	VAL	A	376	14.588			1.00	30.57
	ATOM	560	CG1	VAL	A	376	13.093	-18.122		1.00	33.14
	MOTA	561	CG2	VAL	A	376	15.232	-18.952		1.00	30.79
10	ATOM	562	С	VAL	A	376	14.393	-16.159	1.002	1.00	33.80
	ATOM	563	0	VAL	Α	376	13.653	-15.237	0.661	1.00	34.89
	ATOM	564	N	HIS	A	377	14.500	-16.568	2.261	1.00	33.35
	ATOM	565	CA	HIS	A	377		-15.941	3.329	1.00	32.81
	ATOM	566	CB	HIS	A	377	13.966	-16.694	4.644	1.00	35.24
15	ATOM	567	CG	HIS	Α	377		-15.989	5.851	1.00	40.15
	MOTA	568	CD2	HIS	A	377	14.054		6.946	1.00	40.86
	ATOM	569	ND1	HIS	A	377		-15.703	6.012	1.00	43.08
	ATOM	570	CEl	HIS	А	377	11.913	-15.062	7.154	1.00	42.44
	MOTA	571	NE2	HIS	A	377		-14.922	7.740	1.00	44.85
20	MOTA	572	С	HIS	A	377	14.058	-14.454	3.507	1.00	28.63
	ATOM	573	0	HIS	A	377	13.158	-13.619	3.613	1.00	29.20
	ATOM	574	N	LEU	Α	378	15.343	-14.125	3.544	1.00	24.41
	MOTA	575	CA	LEU	A	378		-12.738	3.721	1.00	23.21
	ATOM	576	CB	LÊU	A	378		-12.650	3.743	1.00	20.98
25	ATOM	577	CG	LEU	A	378		-13.190	5.016	1.00	24.22
	MOTA	578	CD1	LEU	A	378		-13.041	4.924	1.00	21.07
	ATOM	579	CD2	LEU	Α	378		-12.446	6.221	1.00	20.24
	MOTA	580	С	LËU	A	378		-11.827	2.630	1.00	24.78
	MOTA	581	0	LĘŲ	A	378	14.638	-10.766	2.922	1.00	22.09
30	ATOM	582	N	LEU	A	379		-12.242	1.374	1.00	24.13
	MOTA	583	CA	LEU	A	379	14.812	-11.447	0.262	1.00	25.02
	ATOM	584	CB	ΓĒÜ	Ą	379		-12.025		1.00	27.12
	ATOM	585	CG	ΓΈЙ	A	379		-11.600		1.00	24.39
	ATOM	586	CD1	ĻĘŲ	À	379	17.299	-12.557	-2.470	1.00	27.58
35	ATOM	587	CD2	ĻĘŲ	Ä	379	16.679			1.00	29.05
	ATOM	588	С	LEŲ	A	379	13.287	-11.355	0.246	1.00	27.61
	ATOM	589	0	LEU	A	379	12.726	-10.301	-0.062	1.00	26.16
	ATOM	590	N	GĻŲ	A	380	12.616	-12.454	0.576	1.00	25.65
4.0	ATOM	591	CA	GĽÚ	A	380	11.154	-12.471	0.592	1.00	26.85
40	ATOM	592	CB	GĻŲ	Α	380	10.640	-13.882	0.871	1.00	29.38
	ATOM	593	CG	GĻŪ	Α	380	10.718	-14.796	-0.331	1.00	35.58
	ATOM	594	CD	GĽÄ	A	380	10.228	-16.194	-0.025	1.00	39.31
	ATOM	595	OE1	GĻŲ	À	380	10.142	-17.008	-0.967	1.00	42.89
4.5	ATOM	596	OE2	GĽŲ	A	380	9.927	-16.478	1.153	1.00	39.45
45	ATOM	597	C	GLU	A	380	10.604	-11.526	1.649	1.00	25.43
	MOTA	598	0	GLU	Α	380	9.551	-10.925	1.469	1.00	27.75
	ATOM	599	N	CYS	А	381	11.324	-11.400	2.753	1.00	25.57
	MOTA	600	CA	CYS	A	381	10.907	-10.530	3.843	1.00	26.46
50	ATOM	601	CB	CŢŚ	À	381	11.570	-11.000	5.149	1.00	31.46
50	ATOM	602	SG	CYS	A	381	11.305	-9.946	6.623	1.00	45.32
	MOTA	603	C	CYS	A	381	11.262	-9.059	3.589	1.00	24.77
	ATOM	604	0	CYS	A	381	10.516	-8.166	3.975	1.00	25.01
	MOTA	605	N	ALA	A	382	12.377	-8.815	2.903	1.00	22.23
	ATOM	606	CA	AĻA	Α	382	12.855	-7.449	2.681	1.00	21.83
55	ATOM	607	CB	ALA	Α	382	14.319	-7.383	3.095	1.00	21.56
	ATOM	608	С	ALA	Α	382	12.705	-6.778	1.311	1.00	19.78
	ATOM	609	0	ALA	Α	382	12.996	-5.587	1.182	1.00	17.01
	ATOM	610	N	TRP	A	383	12.261	-7.507	0.294	1.00	17.61
	ATOM	611	CA	TRP	Α	383	12.164	-6.915	-1.036	1.00	18.06
60	ATOM	612	CB	TRP	A	383	11.580	-7.928		1.00	20.28
	ATOM	613	CG	TRP	Α	383	10.105	-8.201	-1.919	1.00	20.50

5	ATOM	614	CD2	TRP	A	383		0.049	-7.509 -		1.00	22.48
	ATOM	615	CE2	TRP	A	383		7.836	-8.138 -		1.00	20.41
	MOTA	616	CE3	TRP	Α	383		9.012	-6.420 ·		1.00	22.06
	MOTA	617	CD1	TRP	Α	383	:	9.506	-9.189 ·		1.00	23.38
	ATOM	618	NE1	TRP	Α	383		3.142	-9.159		1.00	22.59
10	MOTA	619	CZ2	TRP	A	383	(6.598	-7.713		1.00	21.98
	ATOM	620	CZ3	TRP	Α	383	•	7.780	-5.998		1.00	25.50
	ATOM	621	CH2	TRP	A	383		6.589	-6.647		1.00	23.11
	MOTA	622	С	TRP	Α	383	1	1.448	-5.564		1.00	19.18
	ATOM	623	0	TRP	Α	383	1	1.972	-4.663	-1.824	1.00	19.27
15	ATOM	624	N	LEU	Α	384	1	0.273	-5.396	-0.567	1.00	18.32
	ATOM	625	CA	LEU	A	384		9.586	-4.118	-0.719	1.00	16.38
	MOTA	626	CB	LEU	Α	384		8.125	-4.218	-0.258	1.00	16.79
	MOTA	627	CG	LEU	A	384		7.211	-3.013	-0.577	1.00	18.39
	ATOM	628	CD1	LEU	Α	384		7.464	-2.485	-1.995	1.00	13.91
20	ATOM	629	CD2	LEU	Α	384		5.750	-3.432	-0.410	1.00	18.38
	ATOM	630	C	LEU	Α	384	1	0.324	-3.027	0.051	1.00	18.80
	ATOM	631	ō	LEŲ	A	384		0.334	-1.870	-0.357	1.00	20.90
	ATOM	632	N	GLU	A	385	1	0.949	-3.404	1.163	1.00	18.61
	ATOM	633	CA	GLU	A	385		1.718	-2.462	1.970	1.00	19.58
25	ATOM	634	CB	GLU	A	385		2.274	-3.154	3.213	1.00	17.43
	MOTA	635	CG	GLU	A	385	1	1.292	-3.237	4.357	1.00	22.92
	ATOM	636	CD	GĻŲ	A	385		1.963	-3.676	5.640	1.00	25.83
	ATOM	637	OE1	GLU	A	385		2.431	-2.799	6.391	1.00	23.69
	ATOM	638	OE2	GLÜ	A	385	1	2.027	-4.897	5.889	1.00	27.64
30	ATOM	639	C	GLÜ	A	385		2.890	-1.934	1.156	1.00	19.46
20	ATOM	640	Ö	GLÜ	A	385		.3.206	-0.743	1.196	1.00	15.04
	ATOM	641	N	IĻĘ	A	386		3.539	-2.842	0.431	1.00	13.32
	ATOM	642	CA	ILE	A	386	1	4.685	-2.484	-0.388	1:00	15.01
	ATOM	643	CB	ILE	A	386		15.475	-3.763	-0.807	1.00	17.43
35	ATOM	644	CG2	ILE	A	386	1	L6.544		-1.849	1.00	17.99
55	ATOM	645	CG1	ILE	A	386	-	16.185	-4.338	0.432	1.00	20.31
	MOTA	646	CD1	ILE	A	386		16.682	-5.766	0.284	1.00	23.97
	ATOM	647	C	ILE	A	386		14.273	-1.645	-1.598	1.00	16.10
	ATOM	648	Ō	ILE	Α	386		14.993	-0.724	-2.004	1.00	17.42
40	ATOM	649	N	LEU	A	387		13.112		-2.167	1.00	17.61
	ATOM	650	CA	LEU	Α	387		12.620	-1.173	-3.304	1.00	18.20
	ATOM	651	CB	LEU	A	387		11.359		-3.882	1.00	17.51
	ATOM	652	CG	LEU	A	387		11.519		-4.747	1.00	26.37
	ATOM	653	CD1	LEU	Α	387		10.173	-3.406	-5.395	1.00	24.63
45	ATOM	654	CD2	LEU	A	387		12.589		-5.808	1.00	21.58
	ATOM	655	c	LEU	Α	387		12.283		-2.838	1.00	17.60
	ATOM	656	Ö	LEU	A	387		12.571		-3.530	1.00	17.15
	MOTA	657	N	MET	A	388		11.677		-1.660		17.65
	ATOM	658	CA	MET	A	388		11.286		-1.121		18.49
50	ATOM	659	CB	MET	A	388		10.302	1.460			19.65
50	ATOM	660	CG	MET	A	388		8.893		-0.435		15.12
	ATOM	661	SD	MET	A	388		7.744				18.73
	ATOM	662	CE	MET	A	388		6.163				
	MOTA	663	C	MET	A	388		12.451		-0.691		
55	ATOM	664	0	MET	A	388		12.417		-0.928		
در		665	Ŋ	ILE	A	389		13.482		-0.064		
	ATOM	666	CA	ILE	A	389		14.604				
	ATOM			ILE	A	389		15.590				
	ATOM	667	CB	ILE	A	389		16.362				
60	ATOM	668 669	CG2 CG1	ILE	A	389		16.556				
00	ATOM			ILE	A			17.373				
	MOTA	670	CD1	1112	A	209		11.3/3	2.030	. 5.000		

5	ATOM	671	C	ILE	λ	389	15 222	2 222 0 000		
•	ATOM	672	0	ILE	A A		15.333	3.322 -0.922	1.00	18.67
	ATOM	673	N	GLY		389	15.813	4.453 -0.970	1.00	19.75
	ATOM	674	CA		A	390	15.410	2.477 -1.943	1.00	20.58
	ATOM	675	CA	GLY	A	390	16.049	2.895 -3.183	1.00	19.33
10	ATOM	676	0	GLY	A	390	15.243	4.021 -3.819	1.00	17.48
10	ATOM			GLY	A	390	15.801	4.994 -4.318	1.00	21.87
		677	N	LEU	A	391	13.920	3.888 -3.787	1.00	19.17
	ATOM	678	CA	LEU	A	391	13.018	4.887 -4.343	1.00	21.50
	ATOM	679	CB	LEU	A	391	11.561	4.420 -4.194	1.00	18.25
15	ATOM	680	CG	LEU	A	391	10.480	5.497 -4.342	1.00	21.98
13	ATOM	681	CD1	LEU	A	391	10.579	6.156 -5.725	1.00	21.39
	ATOM	682	CD2	LEU	Α	391	9.115	4.868 -4.148	1.00	17.15
	ATOM	683	C	LEU	A	391	13.208	6.216 -3.620	1.00	23.27
	ATOM	684	0	LEU	A	391	13.440	7.255 -4.243	1.00	23.60
20	ATOM	685	N	VAL	A	392	13.122	6.170 -2.295	1.00	23.04
20	ATOM	686	CA	VAL	A	392	13.282	7.357 -1.469	1.00	24.42
	ATOM	687	CB	VAL	A	392	13.186	6.993 0.042	1.00	27.38
	ATOM	688	CG1	VAL	A	392	13.733	8.129 0.897	1.00	30.37
	ATOM	689	CG2	VAL	A	392	11.739	6.712 0.414	1.00	23.48
25	ATOM	690	C	VAL	A	392	14.626	8.014 -1.754	1.00	27.55
25	ATOM	691	0	VAL	A	392	14.728	9.242 -1.832	1.00	27.50
	MOTA	692	N	TRP	A	393	15.652	7.186 -1.924	1.00	23.65
	ATOM	693	CA	TRP	A	393	16.999	7.670 -2.204	1.00	24.76
	ATOM	694	CB	TRP	A	393	17.977	6.491 -2.199	1.00	22.86
20	ATOM	695	CG	TRP	A	393	19.287	6.784 -2.857	1.00	25.90
30	ATOM	696	CD2	TRP	A	393	20.341	7.605 -2.339	1.00	28.09
	MOTA	697	CE2	TRP	A	393	21.375	7.612 -3.302	1.00	29.94
	ATOM	698	CE3	TRP	A	393	20.512	8.335 -1.154	1.00	30.20
	ATOM	699	CD1	TRP	A	393	19.710	6.339 -4.077	1.00	26.55
25	ATOM	700	NE1	TRP	A	393	20.963	6.833 -4.351	1.00	30.64
35	ATOM	701	CZ2	TRP	Α	393	22.566	8.323 -3.120	1.00	32.43
	ATOM	702	CZ3	TŔP	À	393	21.698	9.044 -0.971	1.00	34.58
	ATOM	703	CH2	TRP	A	393	22.709	9.030 -1.950	1.00	36.54
	ATOM	704	C	TRP	Α	393	17.082	8.414 -3.547	1.00	25.02
40	ATOM	705	0	TŖP	Α	393	17.767	9.435 -3.650	1.00	20.97
40	ATOM	706	N	ARG	A	394	16.399	7.897 -4.568	1.00	23.06
	MOTA	707	CA	ARG	A	394	16.412	8.531 -5.890	1.00	25.97
	ATOM	708	CB	ARG	Α	394	15.776	7.633 -6.965	1.00	24.05
	ATOM	709	CG	ARG	A	394	16.243	6.195 -7.024	1.00	26.05
15	ATOM	710	CD	ARG	A	394	15.830	5.551 -8.352	1.00	22.70
45	MOTA	711	NE	ARG	À	394	14.443	5.071 -8.363	1.00	20.71
	ATOM	712	CZ	ARG	Α	394	14.053	3.912 -7.841	1.00	21.26
	ATOM	713	NH1	AŖĢ	A	394	14.944	3.108 -7.267	1.00	20.09
	ATOM	714	NH2	ARG	Α	394	12.783	3.544 -7.907	1.00	21.26
50	ATOM	715	С	ARG	Α	394	15.622	9.833 -5.879	1.00	23.40
50	ATOM	716	0	ARG	Α	394	15.889	10.729 -6.677	1.00	28.61
	MOTA	717	N	SER	Α	395	14.638	9.924 -4.988	1.00	26.65
	ATOM	718	CA	SER	A	395	13.776	11.104 -4.902	1.00	27.46
	MOTA	719	CB	SER	A	395	12.395	10.696 -4.382	1.00	26.70
	ATOM	720	OG	SER	A	395	11.916	9.530 -5.029	1.00	22.95
55	ATOM	721	C	SER	Α	395	14.316	12.240 -4.033	1.00	31.45
	ATOM	722	0	SER	Α	395	13.726	13.324 -3.977	1.00	28.11
	ATOM	723	N	MET	Α	396	15.437	11.986 -3.368	1.00	33.83
	ATOM	724	CA	MET	Α	396	16.061	12.954 -2.475	1.00	38.83
	ATOM	725	CB	MET	A	396	17.466	12.483 -2.112	1.00	39.47
60	MOTA	726	CG	MET	Α	396	17.585	11.919 -0.715	1.00	41.37
	ATOM	727	SD	MET	Α	396	19.192	12.262 0.004	1.00	42.20
										- -

								13.996 -1.404 1.00 42.84
5	ATOM	728	CE	MET A	7	396		
,	ATOM	729			Ą	396		14.5.0
	ATOM	730			A,	396	15.637	
		731			A	397	16.794	14.526 -4.166 1.00 42.19
	ATOM				A.	397	16.971	15.831 -4.790 1.00 44.80
	MOTA	732	_		A	397	18.184	15.785 -5.729 1.00 46.02
10	MOTA	733	CB		A	397	17.883	15.189 -7.096 1.00 54.42
	MOTA	734	CG			397	19.117	14.665 -7.810 1.00 59.40
	MOTA	735	CD		A		19.219	13.430 -7.990 1.00 60.63
	ATOM	736	OE1		A	397		15.485 -8.196 1.00 62.71
	MOTA	737	OE2	GLU	A	397	19.980	16.322 -5.554 1.00 42.94
15	MOTA	738	С		Α	397	15.735	17.229 -6.376 1.00 44.68
•	ATOM	739	0	GLU	Α	397	15.830	15.728 -5.280 1.00 40.82
	ATOM	740	N	HIS	A	398	14.579	15.720
	ATOM	741	CA	HIS	Α	398	13.342	10.110
	ATOM	742	CB	HIS	Α	398	12.924	13.043 0.555
20	MOTA	743	CG	HIS	Α	398	13.870	14.886 -8.104 1.00 41.57
20		744	CD2	HIS	A	398	13.904	15.484 -9.318 1.00 39.28
	ATOM		ND1	HIS	A	398	14.940	14.017 -8.074 1.00 41.85
	MOTA	745		HIS	A	398	15.592	14.086 -9.220 1.00 40.88
	MOTA	746	CE1		A	398	14.985	14.969 -9.993 1.00 42.30
	MOTA	747	NE2	HIS		398	12.216	16.332 -4.944 1.00 37.04
25	MOTA	748	C	HIS	A	398	11.282	15.535 -4.864 1.00 36.51
	MOTA	749	0	HIS	A		12.283	17.427 -4.171 1.00 39.19
	MOTA	750	N	PRO	A	399	13.328	18.467 -4.198 1.00 35.36
	MOTA	751	CD	PRO	A	399		17.709 -3.173 1.00 37.10
	MOTA	752	CA	PRO	Α	399	11.243	19.101 -2.654 1.00 37.86
30	MOTA	753	CB	PRO	Α	399	11.603	19.267 -2.963 1.00 35.83
	ATOM	754	CG	PRO	Α	399	13.050	17.663 -3.744 1.00 37.02
	MOTA	755	С	PRO	Α	399	9.828	17:005
	ATOM	756	0	PRO	A	399	9.554	10.245
	ATOM	757	N	GLY	Α	400	8.938	10.551 5.551 1 00 32 12
35	MOTA	758	CA	GLY	Α	400	7.559	10.005
22	ATOM	759	C	GĻŸ	A	400	7.230	13.700
	MOTA	760		GLY	Α	400	6.063	13.344 2.0.
		761		LYS	A	401	8.237	15.112 -5.055 1.00 31.35
	MOTA	762		LYS	A	401	7.972	14.007 -5.966 1.00 30.75
40	MOTA			LYŞ	A	401	8.235	14.430 -7.415 1.00 35.43
40		763		LYS	A	401	8.130	15.927 -7.675 1.00 35.15
	MOTA	764		LYS	A	401	9.096	16.353 -8.774 1.00 36.88
	MOTA	765			A.	401	8.733	17.721 -9.331 1.00 36.71
	MOTA	766		LYS		401	7.295	18.027 -9.116 1.00 34.22
	MOTA	767		LYS	A		8.768	
45		768		LYS	A		9.809	
	MOTA	769		LYS	A		8.256	
	MOTA	770	N C	LEU	A			1 20 20 27
	ATOM	77:	L CA	LĘU	A		8.889	1 00 22 EE
	MOTA	77:	2 CB	LEU	A		7.866	1 007 1 00 24 94
50		77:	3 CG	LEU	Α	402	7.269	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
~	ATOM	77.		LEU	Α	402	6.12	0.303 3.55
	ATOM	77		LEU	A	402	8.35	
	MOTA	77		LEU		402	9.44	8 9.948 -7.414 1.00 28.78
		77		LEU			8.70	9.836 -8.389 1.00 29.98
_	MOTA			LEU			10.76	1 9.770 -7.487 1.00 27.57
5:		77	_	LEU			11.39	3 9.400 -8.744 1.00 2/-1/
	MOTA	77					12.82	5 9.937 -8.816 1.00 26.95
	MOTA	_		LEU			13.40	020 1 00 20 42
	MOTA						14.51	1 10.02
	ATOM					403		
6	MOTA 0					A 403	13.91	.5 0.000 0.01 1.00 24.78
	ATOM	78	4 C	LEU	7 2	A 403	11.41	.7 1.671 0.272

5	ATOM	785	0	LEU.	A	403	12 420	7 257 0 610	3 00	24 62
_	ATOM	786	И	PHE	A	404	12.428 10.306	7.257 -8.619	1.00	24.68
	ATOM	787	CA	PHE	A	404	10.308	7.319 -9.344 5.881 -9.546	1.00	23.11
	ATOM	788	CB	PHE	A	404			1.00	26.93
	ATOM	789	CG	PHE		404	8.826	5.470 -9.946	1.00	27.04
10	ATOM	790	CD1	PHE	A		7.850	5.513 -8.816	1.00	27.89
10	ATOM	791	CD1		A	404	7.028	6.623 -8.631	1.00	26.20
	ATOM	791 792		PHE.	A	404	7.750	4.444 -7.925	1.00	23.10
	ATOM		CE1	PHE	A	404	6.116	6.668 -7.573	1.00	25.29
	ATOM	793 794	CE2	PHE	A	404	6.845	4.481 -6.870	1.00	21.01
15	ATOM		CZ	PHE	A	404	6.026	5.595 -6.693	1.00	22.91
13		795	C	PHE	A	404	11.232	5.507-10.637	1.00	26.04
	ATOM	796	0	PHE	A	404	11.882	4.464-10.578	1.00	27.27
	ATOM	797	N	ALA	A	405	11.348	6.383-11.626	1.00	28.80
	ATOM	798	CA	ALA	A	405	12.271	6.195-12.740	1.00	29.21
20	ATOM	799	CB	ALA	A	405	11.650	5.287-13.806	1.00	26.89
20	ATOM	800	C	ALA	A	405	12.549	7.578-13.317	1.00	30.23
	ATOM	801	0	ALA	A	405	11.770	8.508-13.109	1.00	27.38
	ATOM	802	N	PRO	Α	406	13.672	7.737-14.032	1.00	30.05
	ATOM	803	CD	PRO	A	406	14.712	6.745-14.352	1.00	26.31
25	ATOM	804	CA	PRO	A	406	13.977	9.053-14.604	1.00	32.10
23	ATOM	805	CB	PRO	A	406	15.232	8.800-15.438	1.00	31.28
	ATOM	806	CG	PRO	A	406	15.865	7.602-14.776	1.00	31.44
	ATOM	807	C	PRQ	A	406	12.820	9.589-15.436	1.00	32.58
	ATOM	808	0	PRO	A	406	12.605	10.796-15.507	1.00	32.58
30	ATOM	809	N	ASN	A	407	12.063	8.690-16.053	1.00	32.86
30	ATOM	810	CA	ASN	A	407	10.935	9.119-16.865	1.00	32.78
	ATOM	811	CB	ASŅ	A	407	10.950	8.418-18.228	1.00	34.73
	ATOM	812	CG	ASN	À	407	10.884	6.907-18.121	1.00	35.37
	ATOM	813	OD1	ASN	A	407	11.189	6.317-17.077	1.00	30.24
35	MOTA MOTA	814	ND2	ASŅ	A	407	10.486	6.268-19.215	1.00	34.08
33	ATOM	815	C	ASŅ	A	407	9.605	8.901-16.166	1.00	34.90
	ATOM	816	0	ASN	Ā	407	8.549	8.897-16.798	1.00	36.09
	ATOM	817 818	N	LEU	A	408	9.660	8.724-14.851	1.00	33.56
	ATOM	819	CA CB	LEÚ	A	408	8.452	8.544-14.061	1.00	35.59
40	ATOM	820	CB	LEU	A	408	8.141	7.062-13.851	1.00	33.81
70	ATOM	821	CD1	LEU	A	408	6.696	6.823-13.397	1.00	36.44
	ATOM	822	CD1	LEŬ	A	408	5.746	7.479-14.390	1.00	34.14
	ATOM	823	CD2	LEU LEU	A	408	6.406	5.334-13.287	1,00	32.96
	ATOM	824	0	LEU	A	408	8.607	9.245-12.717	1.00	38.03
45	ATOM	825	N		A	408	8.880	8.614-11.695	1.00	36.38
	ATOM	826	CA	LEŲ LEŲ	A	409	8.441	10.563-12.741	1.00	37.87
	ATOM	827	CB	PEÑ PEÑ	Ä	409	8.548	11.395-11.553	1.00	37.95
	ATOM	828	CG		A	409	9.373	12.636-11.877	1.00	39.52
	ATOM	829		LEU	A	409	10.023	13.399-10.728	1.00	42.46
50	ATOM	830	CD1	LEU	A	409	11.100	12.547-10.082	1.00	43.24
50	ATOM	831	CD2	LEU	A	409	10.614	14.691-11.266	1.00	46.05
	ATOM	832	C	LEU	A	409	7.132	11.792-11.163	1.00	37.13
			0	LEŲ	A	409	6.482	12.546-11.882	1.00	35.70
	ATOM	833	N	LEU	A	410	6.654	11.284-10.030	1.00	35.29
55	ATOM	834	CA	LEU	A	410	5.297	11.576 -9.583	1.00	33.33
دد	ATOM	835	CB	LEU	A	410	4.503	10.277 -9.449	1.00	29.37
	ATOM	836	CG	LEU	A	410	4.645	9.238-10.560	1.00	32.75
	ATOM	837	CD1	LEU	A	410	4.026	7.925-10.104	1.00	29.16
	ATOM	838	CD2	LEU	A	410	3.958	9.744-11.819	1.00	30.70
60	ATOM	839	C	LEU	A	410	5.207	12.332 -8.261	1.00	35.14
00	ATOM	840	0	LEU	A	410	6.078	12.214 -7.400	1.00	36.94
	MOTA	841	N	ASP	Α	411	4.141	13.108 -8.105	1.00	34.76

5 ATOM 843 CR ASP A 411 3,733 IS.341 -7.144 1.00 40.02 ATOM 845 CR ASP A 411 2.727 IS.645 -7.928 1.00 41.32 ATOM 846 CD ASP A 411 2.471 IS.645 -7.928 1.00 45.01 ATOM 845 CD ASP A 411 2.471 IS.645 -7.928 1.00 45.01 ATOM 846 CD ASP A 411 2.383 IS.341 -7.144 1.00 45.01 ATOM 846 CD ASP A 411 2.383 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.383 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.933 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.933 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.933 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.933 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.933 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.935 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 411 2.935 IS.341 -7.144 1.00 45.01 ATOM 849 CM ASP A 412 2.727 IS.341 -7.144 1.00 35.99 ATOM 855 CD ARG A 412 1.350 IS.341 -7.940 IS.00 35.99 ATOM 855 CD ARG A 412 0.562 IS.168 -2.870 IS.00 37.75 ATOM 855 CD ARG A 412 0.562 IS.168 -2.870 IS.00 40.45 ATOM 855 CM ARG A 412 -0.261 IS.242 -0.577 IS.00 40.45 ATOM 855 CM ARG A 412 -0.261 IS.242 -0.344 IS.340 -0.34 IS.340 ATOM 855 CM ARG A 412 -2.150 IS.346 -0.577 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 855 CM ARG A 412 -2.150 IS.340 IS.00 40.82 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.110 IS.00 40.82 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.82 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.82 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.85 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.85 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.85 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.85 ATOM 850 CM ASM A 413 -1.151 IS.351 IS.353 -7.710 IS.00 40.85 ATOM 850 CM ASM A 413 -1.1451 IS.351 IS.351 IS.00 40.85 ATOM 850 CM ASM A 413 -1.1						Α.	1 1	3.933 13.843 -6.873 1.00 35.40
ATOM 844 CG ASP A 411	5	MOTA	842		ASP A			3 733 15.341 -7.144 1.00 40.02
ATOM 845 ODI ASP A 411		MOTA		_				2 471 15.645 -7.928 1.00 41.32
ATOM 845 ODI ASP A 411 2.383 16.764 -8.474 1.00 45.01 ATOM 840 ODI ASP A 411 2.737 13.234 -6.179 1.00 36.10 36.10 ATOM 840 N ASP A 411 2.033 12.395 -6.762 1.00 34.08 ATOM 849 N ARG A 412 1.375 13.099 -4.169 1.00 35.99 ATOM 850 CA ARG A 412 1.375 13.099 -4.169 1.00 39.75 ATOM 851 CB ARG A 412 0.562 15.168 -2.870 1.00 40.49 ATOM 853 CD ARG A 412 0.562 15.168 -2.870 1.00 40.65 ATOM 853 CD ARG A 412 0.562 15.168 -2.870 1.00 40.65 ATOM 853 CD ARG A 412 0.562 15.168 -2.870 1.00 40.65 ATOM 853 CD ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 855 CZ ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 855 NH1 ARG A 412 -0.261 15.754 -1.042 1.00 40.82 ATOM 857 NH2 ARG A 412 -0.261 15.754 -1.024 1.00 40.82 ATOM 858 C ARG A 412 -0.261 15.754 -1.024 1.00 40.82 ATOM 858 C ARG A 412 -0.261 15.754 -1.024 1.00 40.82 ATOM 858 C ARG A 412 -0.261 13.986 0.438 1.00 38.32 ATOM 858 C ARG A 412 -0.775 12.001 -0.705 10.00 40.99 ATOM 859 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 859 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 860 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 861 CA ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 864 ODI ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 865 ND2 ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 N ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 N ASN A 413 -1.739 16.718 -6.6687 1.00 49.43 ATOM 868 N GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 867 C GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 868 N GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 867 C GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 867 C GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 867 C GIM A 414 -0.703 11.448 -8.995 1.00 47.55 ATOM 867 C GIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM A 414 -0.907 10.163 -8.111 1.00 40.43 ATOM 870 C BIM		MOTA						1 570 14.785 -8.001 1.00 45.03
ATOM 846 ODZ ASP A 411 2.727 13.234 -6.179 1.00 36.10 10 10 ATOM 848 O ASP A 411 2.033 12.395 -6.762 1.00 34.08 ATOM 849 N ARG A 412 1.260 13.824 -2.825 1.00 39.37 ATOM 850 CA ARG A 412 1.260 13.824 -2.825 1.00 39.37 ATOM 850 CD ARG A 412 0.552 15.68 -2.870 1.00 40.49 ATOM 851 CD ARG A 412 0.454 15.736 -1.465 1.00 40.49 ATOM 851 CD ARG A 412 0.454 15.736 -1.465 1.00 40.45 ATOM 855 CZ ARG A 412 0.454 15.736 -1.465 1.00 40.45 ATOM 855 CZ ARG A 412 0.454 15.736 -1.465 1.00 40.45 ATOM 855 CZ ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 855 CD ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 850 ARG A 412 -0.261 14.826 -0.577 1.00 40.45 ATOM 850 ARG A 412 -0.261 14.826 -0.577 1.00 40.48 ATOM 850 ARG A 412 -0.261 14.826 -0.577 1.00 40.48 ATOM 850 ARG A 412 -0.261 14.826 -0.577 1.00 40.48 ATOM 850 ARG A 412 -0.261 14.826 -0.577 1.00 40.48 ATOM 850 ARG A 412 -0.198 14.119 -5.717 1.00 41.64 ATOM 850 ARG A 412 -0.198 14.119 -5.717 1.00 41.64 ATOM 860 ARG A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 860 ARG		MOTA						2 383 16.764 -8.474 1.00 45.01
10		MOTA	846					2 727 13.234 -6.179 1.00 36.10
ATOM 848 O ASP A 412	10	MOTA	847					5 7 5 7 5 7 6 7 6 7 6 8
ATOM 859 CA ARG A 412 1.375 13.099 -4.169 1.00 39.37 ATOM 851 CB ARG A 412 1.260 13.824 -2.825 1.00 39.37 ATOM 852 CG ARG A 412 0.552 15.168 -2.870 1.00 40.49 ATOM 853 CD ARG A 412 0.552 15.168 -2.870 1.00 40.49 ATOM 853 CD ARG A 412 0.552 15.168 -2.870 1.00 40.49 ATOM 853 CD ARG A 412 0.552 15.736 -1.465 1.00 40.65 ATOM 855 NE ARG A 412 -0.261 14.826 -0.577 1.00 42.84 ATOM 856 NH1 ARG A 412 -0.261 14.826 -0.577 1.00 42.84 ATOM 857 NH2 ARG A 412 -0.316 15.736 -1.045 1.00 40.82 ATOM 858 NH2 ARG A 412 -0.1574 14.855 -0.384 1.00 40.82 ATOM 859 NH2 ARG A 412 -0.775 12.201 -4.706 1.00 39.80 ATOM 850 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 860 N ASN A 413 -1.458 14.215 -6.440 1.00 43.19 ATOM 861 CA ASN A 413 -1.458 14.215 -6.440 1.00 43.19 ATOM 863 CG ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 865 ND2 ASN A 413 -1.518 15.533 -7.210 1.00 40.82 ATOM 865 ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 865 ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 867 O ASN A 413 -1.23 17.876 -6.687 1.00 49.43 ATOM 868 N GIN A 414 -0.700 12.577 -8.010 1.00 42.82 ATOM 867 O ASN A 413 -1.673 13.044 -7.385 1.00 44.73 ATOM 869 CA GIN A 414 -0.700 12.577 -8.010 1.00 42.82 ATOM 870 CB GIN A 414 -0.700 12.577 -8.010 1.00 55.91 ATOM 870 CB GIN A 414 -0.700 11.377 -9.741 1.00 47.52 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 871 CG GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 873 OEI GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 55.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 870 CB GIN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 880 CB CB LYS A 416 -5.992 13.994 -3.898 1.00 42.33 ATOM 888 CB CB LYS A 416 -5.992 13.994 -3.898 1.00 40.80 ATOM 888 CB CB LYS A 416 -5.		MOTA	848			_		200 7 00 7 00
ATOM 850 CB ARG A 412		ATOM	849					1 375 13.099 -4.169 1.00 39.37
ATOM 851 CB ARG A 412 0.562 15.168 -2.870 1.00 40.49 ATOM 853 CD ARG A 412 0.454 15.736 -1.465 1.00 40.65 ATOM 854 NE ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 856 NH1 ARG A 412 -0.261 14.826 -0.577 1.00 40.82 ATOM 857 NH2 ARG A 412 -0.2150 13.986 0.438 1.00 39.80 ATOM 858 C ARG A 412 -0.775 12.201 -4.706 1.00 39.80 ATOM 859 C ARG A 412 -0.775 12.201 -4.706 1.00 39.92 ATOM 850 N ASN A 413 -1.458 14.215 -6.440 1.00 41.64 ATOM 850 C ARG A 412 -0.775 12.201 -4.706 1.00 43.19 ATOM 850 C ARG A 412 -0.775 12.201 -4.706 1.00 43.19 ATOM 850 N ASN A 413 -1.458 14.215 -6.440 1.00 44.82 ATOM 850 C ARG A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 850 C ARG A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 850 ND1 ASN A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 866 N ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 N ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 N GLN A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 869 CA GLN A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 870 CB GLN A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 870 CB GLN A 414 -0.570 11.448 -8.925 1.00 47.52 ATOM 871 CG GLN A 414 -0.570 11.448 -8.925 1.00 47.52 ATOM 872 CD GLN A 414 -0.570 11.448 -8.925 1.00 50.47 ATOM 874 NE2 GLN A 414 -0.970 10.163 -8.141 1.00 43.21 ATOM 875 C GLN A 414 -0.970 10.163 -8.141 1.00 43.21 ATOM 876 C GLN A 414 -0.970 10.163 -8.141 1.00 43.21 ATOM 878 CA GLY A 415 -0.836 8.992 -6.040 1.00 40.33 ATOM 886 CC LYS A 416 -5.212 10.996 -5.704 1.00 45.33 ATOM 887 CC GLY A 415 -0.836 8.992 -6.040 1.00 40.33 ATOM 888 CC LYS A 416 -5.212 10.996 -5.704 1.00 45.53 ATOM 889 CC LYS A 416 -5.212 10.996 -5.704 1.00 45.53 ATOM 889 CC LYS A 416 -5.227 8.793 -1.00 47.72 ATOM 889 CC CYS A 417 -4.566 9.613 -1.476 -2.809 1.00 47.42 ATOM 889 CC CYS A 417 -4.506 9.643 -1.160 9.4391 1.00 45.50 ATOM 889 CC CYS A 417 -6.220 5.794 -9.159 1.00 47.42 ATOM 889 CC CYS A 417 -6.200 5.794 -9.159 1.00 47.42 ATOM 889 CC CYS A 417 -6.200 5.79		MOTA						
15 ATOM 852 CG ARG A 412 0.454 15.736 -1.465 1.00 40.65 ATOM 854 NE ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 854 NE ARG A 412 -1.574 14.855 -0.384 1.00 42.84 ATOM 856 NH1 ARG A 412 -2.150 13.966 0.438 1.00 38.32 ATOM 857 NB ARG A 412 -2.150 13.966 0.438 1.00 38.32 ATOM 859 N ARS A 413 -0.755 12.001 -4.706 1.00 39.80 ATOM 860 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 860 N ASN A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 860 N ASN A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 860 N ASN A 413 -1.518 15.533 -7.210 1.00 46.44 ATOM 860 N ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 860 N ASN A 413 -1.518 15.533 -7.210 1.00 48.05 ATOM 865 ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 865 ND2 ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 N ASN A 413 -1.213 17.876 -6.687 1.00 49.43 ATOM 866 N ASN A 413 -1.213 17.876 -6.687 1.00 41.48 ATOM 869 N GLM A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 867 C G GLM A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 867 C G GLM A 414 -0.600 12.577 -8.010 1.00 47.52 ATOM 870 C G GLM A 414 -0.572 12.088-11.049 1.00 50.47 ATOM 871 C G GLM A 414 -0.572 12.088-11.049 1.00 50.47 ATOM 873 OEI GLM A 414 -0.572 12.088-11.049 1.00 50.47 ATOM 875 C GLM A 414 -0.572 12.088-11.049 1.00 50.47 ATOM 875 C GLM A 414 -0.970 11.68 6.860 1.00 42.33 ATOM 879 C GLM A 414 -0.970 10.68 6.913 1.00 42.33 ATOM 879 C GLM A 414 -0.970 10.68 6.913 1.00 42.33 ATOM 879 C GLM A 414 -0.970 10.68 6.913 1.00 42.34 ATOM 879 C GLM A 414 -0.970 10.68 6.913 1.00 42.35 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.90 1.00 44.73 ATOM 870 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.910 1.00 42.33 ATOM 880 C GLM A 414 -0.970 10.68 6.90		MOTA						0.562 15.168 -2.870 1.00 40.49
ATOM 854 NE ARG A 412 -0.261 14.826 -0.577 1.00 37.48 ATOM 856 NEL ARG A 412 -1.574 14.855 -0.381 1.00 42.84 ATOM 856 NH1 ARG A 412 -2.316 15.754 -1.024 1.00 40.82 ATOM 856 NH2 ARG A 412 -2.315 15.754 -1.024 1.00 40.82 ATOM 857 NH2 ARG A 412 -2.150 13.986 0.438 1.00 38.32 ATOM 858 C ARG A 412 -0.775 12.201 -4.706 1.00 39.80 ATOM 860 N ASN A 413 -0.775 12.201 -4.706 1.00 43.19 ATOM 861 CA ASN A 413 -1.518 14.19 -5.717 1.00 41.64 ATOM 862 CB ASN A 413 -1.518 15.533 -7.210 1.00 43.19 ATOM 863 CG ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 863 CG ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 866 C ASN A 413 -1.673 13.044 -7.385 1.00 41.48 ATOM 866 C ASN A 413 -1.673 13.044 -7.385 1.00 41.48 ATOM 866 C ASN A 414 -0.703 11.448 -8.925 1.00 44.73 ATOM 866 N GLN A 414 -0.703 11.448 -8.925 1.00 44.73 ATOM 870 CB GLN A 414 -0.703 11.448 -8.925 1.00 44.73 ATOM 873 OEI GLN A 414 -0.703 11.448 -8.925 1.00 42.82 ATOM 873 OEI GLN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 876 C GLN A 414 -0.970 10.163 -8.141 1.00 56.91 ATOM 877 N GLY A 415 -0.618 1.00 47.52 ATOM 878 CA GLY A 415 -0.618 1.00 47.52 ATOM 880 O GLY A 415 -0.836 8.92 -6.040 1.00 40.80 ATOM 880 C GLY A 415 -0.836 8.92 -6.040 1.00 40.80 ATOM 880 C GLY A 415 -0.618 1.00 47.777 1.00 50.95 ATOM 887 NZ LYS A 416 -5.227 1.096 -5.704 1.00 47.32 ATOM 888 C LYS A 416 -5.227 1.096 -5.704 1.00 47.32 ATOM 888 C C LYS A 416 -5.227 1.096 -5.704 1.00 47.32 ATOM 889 O N CYS A 417 -3.916 9.493-11.168 1.00 49.59 ATOM 889 C CYS A 417 -3.916 9.493-11.168 1.00 49.59 ATOM 889 C CYS A 417 -3.916 9.493-11.168 1.00 49.	15	MOTA	852					0 454 15,736 -1.465 1.00 40.65
ATOM 854 NE ARG A 412 -1.574 14.855 -0.384 1.00 42.84 ATOM 856 NH1 ARG A 412 -2.316 15.754 -1.024 1.00 40.82 ATOM 857 NH2 ARG A 412 -2.150 13.986 0.438 1.00 39.80 ATOM 858 C ARG A 412 -0.034 13.108 -4.889 1.00 39.80 ATOM 859 O ARG A 412 -0.775 12.201 -4.706 1.00 39.92 ATOM 850 N ASN A 413 -0.198 14.119 -5.717 1.00 41.64 ATOM 861 CA ASN A 413 -1.458 14.215 -6.440 1.00 41.64 ATOM 862 CB ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 863 CG ASN A 413 -1.518 15.533 -7.210 1.00 47.86 ATOM 864 OD1 ASN A 413 -1.233 17.876 -6.687 1.00 47.86 ATOM 865 ND2 ARN A 413 -1.233 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.233 17.876 -6.687 1.00 49.43 ATOM 866 C ASN A 413 -1.233 17.876 -6.687 1.00 49.43 ATOM 868 N GIN A 414 -0.600 12.577 -8.010 1.00 42.82 ATOM 868 N GIN A 414 0.585 11.307 -9.741 1.00 45.65 ATOM 870 CB GIN A 414 0.585 11.307 -9.741 1.00 50.47 ATOM 871 CG GIN A 414 0.572 12.088-11.049 1.00 50.47 ATOM 873 OB1 GIN A 414 0.585 11.307 -9.741 1.00 50.47 ATOM 874 NB2 CD GIN A 414 0.572 12.088-11.049 1.00 50.47 ATOM 875 C GIN A 414 -0.970 11.348 8.925 1.00 42.33 ATOM 876 N GIN A 414 -0.970 11.368 -6.800 1.00 42.82 ATOM 877 N GLY A 415 -0.836 8.992 -6.040 1.00 42.33 ATOM 878 C GIN A 414 -0.970 10.163 -8.141 1.00 53.68 ATOM 879 C GIV A 415 -0.836 8.992 -6.040 1.00 40.43 ATOM 878 C GIV A 415 -0.836 8.992 -6.040 1.00 44.34 ATOM 878 C GIV A 415 -0.836 8.992 -6.040 1.00 44.34 ATOM 878 C GIV A 415 -0.836 8.992 -6.040 1.00 44.34 ATOM 888 C G LYS A 416 -5.212 10.996 -5.704 1.00 45.65 ATOM 889 C LYS A 416 -5.212 10.996 -5.704 1.00 45.65 ATOM 889 C CYS A 417 -4.506 7.992 1.00 37.83 ATOM 889 C CYS A 417 -5.066 7.992 1.00 45.51 ATOM 889 C CYS A 417 -5.066 7.992 1.00 45.51 ATOM 889 C CYS A 417 -5.373 6.452 -8.752 1.00 47.42 ATOM 889 C CYS A 417 -5.066 7.992 1.00 45.51 ATOM 889 C CYS A 417 -5.373 6.452 -8.752 1.00 47.18 ATOM 889 C CYS A 417 -5.373 6.452 -7.331 1.00 45.51		MOTA						0 361 14.826 -0.577 1.00 37.48
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ATOM 869 CA GLN A 414 0.585 11.307 -9.741 1.00 47.52 ATOM 871 CG GLN A 414 0.572 12.088-11.049 1.00 50.47 ATOM 871 CG GLN A 414 1.914 12.713-11.375 1.00 53.91 ATOM 873 OE1 GLN A 414 2.309 12.637-12.641 1.00 56.91 ATOM 875 C GLN A 414 -0.970 10.163 -8.141 1.00 42.33 ATOM 876 O GLN A 414 -0.970 10.163 -8.141 1.00 42.33 ATOM 877 N GLY A 415 -0.618 10.168 -6.860 1.00 41.97 ATOM 878 CA GLY A 415 -0.618 10.168 -6.860 1.00 40.80 ATOM 879 C GLY A 415 -2.306 8.720 -5.804 1.00 40.80 ATOM 881 N LYS A 416 -3.129 9.748 -5.978 1.00 42.16 ATOM 882 CA LYS A 416 -4.566 9.613 -5.779 1.00 44.34 ATOM 883 CB LYS A 416 -4.566 9.613 -5.779 1.00 44.34 ATOM 885 CD LYS A 416 -4.761 11.819 -4.510 1.00 45.65 ATOM 885 CD LYS A 416 -4.761 11.819 -4.510 1.00 47.42 ATOM 886 CE LYS A 416 -4.761 11.819 -4.510 1.00 45.33 ATOM 888 C LYS A 416 -5.212 10.996 -5.704 1.00 45.65 ATOM 887 NZ LYS A 416 -5.212 10.996 -5.704 1.00 45.65 ATOM 888 C LYS A 416 -5.227 8.793 -6.886 1.00 45.33 ATOM 889 O LYS A 416 -5.227 8.793 -6.886 1.00 45.33 ATOM 889 O LYS A 416 -5.227 8.793 -6.886 1.00 45.33 ATOM 889 O LYS A 416 -5.227 8.793 -6.886 1.00 45.33 ATOM 889 C LYS A 416 -5.227 8.793 -6.886 1.00 45.33 ATOM 889 O LYS A 416 -6.339 8.299 -6.714 1.00 45.50 ATOM 889 C CYS A 417 -4.062 7.902-10.305 1.00 45.55 ATOM 891 CA CYS A 417 -5.366 7.890 -9.148 1.00 46.50 ATOM 893 SG CYS A 417 -5.366 7.890 -9.148 1.00 46.50 ATOM 893 SG CYS A 417 -5.373 6.452 8.793 -6.886 1.00 47.18 ATOM 894 C CYS A 417 -5.373 6.452 8.793 -6.875 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.793 -6.875 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.793 -1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.793 -1.00 46.50 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452 8.752 1.00 42.75		MOTA						0 703 11 448 -8.925 1.00 44.73
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ATOM 873 OE1 GLN A 414 2.309 12.637-12.641 1.00 56.91 ATOM 874 NE2 GLN A 414 -0.970 10.163-8.141 1.00 43.21 ATOM 875 C GLN A 414 -1.491 9.193 -8.682 1.00 42.33 ATOM 876 O GLN A 415 -0.618 10.168-6.860 1.00 41.97 ATOM 877 N GLY A 415 -0.836 8.992 -6.040 1.00 40.43 ATOM 878 CA GLY A 415 -2.306 8.720-5.804 1.00 40.80 ATOM 880 O GLY A 415 -2.696 7.601-5.472 1.00 37.83 ATOM 881 N LYS A 416 -3.129 9.748-5.978 1.00 42.16 ATOM 882 CA LYS A 416 -4.566 9.613-5.779 1.00 44.34 ATOM 883 CB LYS A 416 -5.212 10.996-5.704 1.00 45.65 ATOM 885 CD LYS A 416 -4.761 11.819-4.510 1.00 47.42 ATOM 886 CE LYS A 416 -4.761 11.819-4.510 1.00 47.42 ATOM 886 CE LYS A 416 -5.992 13.924-3.898 1.00 53.25 ATOM 887 NZ LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 888 C LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 889 O LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 889 C LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 886 CE LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 887 NZ LYS A 416 -5.212 10.996-5.704 1.00 45.33 ATOM 888 C LYS A 416 -5.992 13.924-3.898 1.00 53.25 ATOM 886 CE LYS A 416 -5.227 8.793-6.886 1.00 45.33 ATOM 889 C LYS A 416 -5.227 8.793-6.886 1.00 45.33 ATOM 889 C CYS A 417 -5.066 7.890-9.148 1.00 46.50 ATOM 890 N CYS A 417 -5.066 7.890-9.148 1.00 46.25 ATOM 893 SG CYS A 417 -5.373 6.452-8.752 1.00 47.18 ATOM 894 C CYS A 417 -5.373 6.452-8.752 1.00 47.18 ATOM 895 O CYS A 417 -5.373 6.452-8.752 1.00 47.18 ATOM 896 N VAL A 418 -4.866 4.612-7.232 1.00 42.75 ATOM 896 N VAL A 418 -4.866 4.612-7.232 1.00 42.75	35							2 591 13.257-10.501 1.00 53.68
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## ATOM ## ATO								-0.618 10.168 -6.860 1.00 41.97
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ATOM 879 C GLY A 415 ATOM 880 O GLY A 415 ATOM 881 N LYS A 416 ATOM 882 CA LYS A 416 ATOM 882 CA LYS A 416 ATOM 883 CB LYS A 416 ATOM 884 CG LYS A 416 ATOM 885 CD LYS A 416 ATOM 886 CE LYS A 416 ATOM 887 NZ LYS A 416 ATOM 888 C LYS A 416 ATOM 888 C LYS A 416 ATOM 888 C LYS A 416 ATOM 889 O LYS A 416 ATOM 889 O LYS A 416 ATOM 889 C LYS A 416 ATOM 890 N CYS A 417 ATOM 891 CA CYS A 417 ATOM 892 CB CYS A 417 ATOM 893 SG CYS A 417 ATOM 894 C CYS A 417 ATOM 895 O CYS A 417 ATOM 896 N VAL A 418 ATOM 896 N VAL A 418 ATOM 897 CA VAL A 418 ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM					•			2 306 8 720 -5.804 1.00 40.80
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55 ATOM 892 CB CYS A 417 ATOM 893 SG CYS A 417 ATOM 894 C CYS A 417 ATOM 895 O CYS A 417 ATOM 896 N VAL A 418 ATOM 897 CA VAL A 418 -3.525 3.841-7.206 1.00 42.45								-4 062 7.902-10.305 1.00 49.29
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60 ATOM 897 CA VAL A 110 -3.525 3.841 -7.206 1.00 42.45		MOTA	89					1 00 42 75
ATOM 898 CB VAL A 418 -3.323 3.525	6	MOTA 0	89	_				-4.860 1.012 - 206 1 00 42 45
		ATOM	1 89	98 CI	3 VAL	A	418	

5	3.004				_					
3	ATOM	899	CG1	VAL	Α	418	-3.670	2.563 -6.410	1.00	40.22
	ATOM	900	CG2	VAL	Α	418	-3.071	3.538 -8.634	1.00	38.03
	ATOM	901	С	ΛŸΪ	A	418	-5.441	4.714 -5.818	1.00	41.46
	ATOM	902	0	VAL	Α	418	-4.883	5.400 -4.963	1.00	42.08
	ATOM	903	N	GLU	Α	419	-6.559	4.036 -5.579	1.00	40.95
10	ATOM	904	CA	GLU	A	419	-7.223	4.073 -4.275	1.00	42.51
	ATOM	905	CB	GLU	A	419	-8.536	3.282 -4.333	1.00	44.52
	ATOM	906	CG	GLU	Α	419	-9.010	2.751 -2.984	1.00	50.42
	ATOM	907	CD	GLU	A	419	-10.413	2.168 -3.035	1.00	54.38
	ATOM	908	OE1	GLU	A	419	-10.582	1.059 -3.590	1.00	
15	ATOM	909	OE2	GLU	A	419	-11.347			54.09
	ATOM	910	c	GLU	A	419		2.820 -2.516	1.00	57.90
	ATOM	911	o	GLU			-6.370	3.552 -3.121	1.00	41.11
	ATOM	912	N	GLY	A	419	-5.955	2.393 -3.116	1.00	39.42
	ATOM	913	CA		A	420	-6.129	4.419 -2.140	1.00	40.53
20	ATOM			GLY	A	420	-5.346	4.049 -0.973	1.00	37.61
20		914	С	GLY.	A	420	-3.854	4.258 -1.140	1.00	37.01
	ATOM	915	0	GLY	A	420	-3.088	4.105 -0.190	1.00	32.59
	ATOM	916	N	MET	Α	421	-3.444	4.623 -2.350	1.00	36.21
	ATOM	917	CA	MEŢ	Α	421	-2.035	4.825 -2.656	1.00	36.02
0.5	ATOM	918	CB	MET	Α	421	-1.799	4.607 -4.160	1.00	32.84
25	ATOM	919	CG	MÉT	A	421	-0.351	4.754 -4.617	1.00	35.82
	ATOM	920	SD	MET	Α	421	0.806	3.611 -3.812	1.00	35.57
	ATOM	921	CE	MET	A	421	0.881	2.294 -5.005	1.00	32.51
	MOTA	922	С	MET	À	421	-1.474	6.180 -2.226	1.00	34.93
	MOTA	923	0	MET	Ą	421	-0.275	6.294 -1.985	1.00	35.17
30	ATOM	924	N	VAL	À	422	-2.319	7.205 -2.118	1.00	33.97
	ATOM	925	CA	VAL	A	422	-1.823	8.520 -1.708	1.00	31.29
	ATOM	926	CB	VAL	A	422	-2.927	9.607 -1.766	1.00	33.14
	ATOM	927	CG1	VAL	A	422	-3.823	9.535 -0.533	1.00	30.14
	ATOM	928	CG2	VAL	A	422	-2.279	10.982 -1.854		
35	ATOM	929	C	VAL	A	422	-1.231	8.498 -0.296	1.00	30.08
	ATOM	930	Ō	VAL	A	422	-0.274		1.00	32.64
	ATOM	931	N	GLU	A	423	-1.803		1.00	28.41
	ATOM	932	CA	GLÜ	A	423		7.670 0.571	1.00	31.53
	ATOM	933	CB	GĽÚ	A	423	-1.311	7.558 1.935	1.00	35.99
40	ATOM	934	CG	GLÜ	À		-2.190	6.594 2.737	1.00	40.37
	ATOM	935	CD	GTÜ	A	423	-3.588	7.129 3.043	1.00	49.41
	ATOM	936	OE1			423	-4.438	7.336 1.795	1.00	52.38
	ATOM	937	OE2	GLŲ	A	423	-5.349	8.188 1.835	1.00	56.91
	ATOM	938	C	GLŲ	A	423	-4.200	6.652 0.776	1.00	54.53
45	ATOM	939	-	GLU	À	423	0.127	7.043 1.886	1.00	34.83
43	ATOM		0	GĽÜ	Ä	423	1.007	7.552 2.581	1.00	31.85
	ATOM	940	N	ILE	A	424	0.369	6.038 1.050	1.00	30.17
		941	CA	ILE	Α	424	1.711	5.488 0.929	1.00	28.99
	ATOM	942	CB	ILE	Α	424	1.696	4.195 0.109	1.00	30.96
50	ATOM	943	CG2	ILE	A	424	3.108	3.588 0.068	1.00	27.20
30	ATOM	944	CG1	ILE	Α	424	0.671	3.230 0.725	1.00	30.77
	ATOM	945	CD1	ILE	Α	424	0.810	1.787 0.291	1.00	34.69
	ATOM	946	С	ILE	Α	424	2.700	6.483 0.312	1.00	28.21
	ATOM	947	0	ILE	À	424	3.856	6.551 0.735	1.00	28.48
	ATOM	948	N	PHE	A	425	2.253	7.260 -0.675	1.00	27.68
55	MOTA	949	CA	PHE	Α	425	3.119	8.253 -1.315	1.00	27.30
	ATOM	950	CB	PHE	A	425	2.381	8.958 -2.458	1.00	26.36
	ATOM	951	CG	PHE	A	425	2.538	8.289 -3.798		
	MOTA	952	CD1	PHE	A	425	2.619	9.050 -4.958	1.00	27.22
	ATOM	953	CD2	PHE	A	425			1.00	27.36
60	ATOM	954	CE1	PHE	À	425	2.566 2.721	6.900 -3.905	1.00	27.89
	ATOM	955	CE2	PHE	A	425		8.443 -6.207	1.00	29.63
			4			743	2.668	6.282 -5.149	1.00	27.28

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				_			2.745	7.056 -6.303 1.00 27.63
5	ATOM	956		PHE P		25	3.591	9.306 -0.312 1.00 25.66
	MOTA	957		PHE F		125	4.757	9.713 -0.328 1.00 26.33
	MOTA	958	0	 .		125	2.680	9.746 0.552 1.00 27.92
	ATOM	959	N			126		10.759 1.570 1.00 28.88
	ATOM	960	CA	ASP I		426	2.984	11.102 2.369 1.00 32.58
10	ATOM	961	CB	ASP 2		426	1.721	12.034 1.613 1.00 37.47
10	ATOM	962	CG	ASP .		426	0.781	12.039 1.925 1.00 37.72
	MOTA	963	OD1	ASP		426	-0.432	14.039 1.000 26 25
	MOTA	964	OD2	ASP	-	426	1.253	12.756 0.720 = 20 20 96
	ATOM	965	С	ASP	A	426	4.071	10.278 2.332
15	ATOM	966	0		A	426	4.974	11.030 2.300
15		967	N	MET	A	427	3.978	9.022 2.31
	MOTA	968	CA	MET	A	427	4.981	0.400 3.000
	MOTA	969	CB	MET	A	427	4.567	7.070 1.30
	ATOM	970	CG	MET	A	427	3.385	7.072 3.23
	ATOM		SD	MET	A	427	3.153	3.405 0.000
20	MOTA	971	CE	MET	A	427	2.173	4.03, 1
	MOTA	972	CE	MET	Α	427	6.321	8.410 3.220
	MOTA	973		MET	A	427	7.363	8.760 3.689 1.00 22.19
	MOTA	974	0		A	428	6.285	7.985 1.868 1.00 21.75
	MOTA	975	N	LEU	A	428	7.506	7.892 1.075 1.00 22.91
25	MOTA	976	CA	LEU	A	428	7.202	7.252 -0.287 1.00 18.47
	MOTA	977	CB	LEU	Ā	428	6.910	5.747 -0.176 1.00 19.24
	MOTA	978	CG	LEU	A	428	6.278	5.222 -1.468 1.00 16.82
	MOTA	979	CD1	LĘŲ	A	428	8.204	5.010 0.131 1.00 16.23
	MOTA	980	CD2	r <u>ęń</u>		428	8.148	9.269 0.902 1.00 23.98
30	MOTA	981	C	ĽĘŰ	A	428	9.366	9.416 1.034 1.00 23.06
	MOTA	982	0	LEU	A	429	7.328	10.281 0.628 1.00 23.91
	MOTA	983	N	ΓΕ̈́Ω	A	429	7.837	11.642 0.462 1.00 26.29
	MOTA	984		Ŀ <u>ĔÜ</u>	Ą		6.714	12.571 -0.003 1.00 27.47
	ATOM	985		ΓΈΩ	A	429	6.331	12 411 -1.476 1.00 30.78
35	MOTA	986		ΓĔЙ	A	429	5.022	12 139 -1.751 1.00 34.75
	MOTA	987		LEŲ	A	429	7.449	12 952 -2.350 1.00 31.96
	MOTA	988			Ä	429	8.425	12,166 1.776 1.00 25.83
	MOTA	989) C	ΓΈΩ	À	429	9.482	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
	MOTA	990	0	ΓĔЙ	A	429	7.734	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
40		993	L N	ALA	A	430		12 333 4.185 1.00 26.11
	MOTA	992	2 CA	ALA	Α	430	8.203	
	MOTA	99:	3 CB	AنيِّA		430	7.214	1 11.000 - 4 460 1 00 25.01
	ATOM	99	4 C	AĻĄ		430	9.57	7 1:00 24 31
	ATOM	99	5 0	ĄĹĄ	. A	430	10.45	3 12.305
4:				THR		431	9.76	7 10.100
-1.	ATOM			THR	, A	431	11.04	6 9.025 2.00 21 36
	MOTA			THR	Į Ā		10.97	3 8.323 3.502 1 00 20 27
	ATOM				A	431	9.92	4 7.727 1.00 1.00 19.99
	ATOM		00 CG		A S	431	12.29	7.633 4.200 1 00 23 73
_			01 C	THE	į A	431	12.10	13 10.477 5.225
)	•		02 0	THE		431	13.23	14 10.007 3.00 1 00 24 32
	ATOM		03 N	SEF		432	11.73	20.013 2 1 00 26 96
	MOTA		004 CA			432	12.67	76 11.475 1.502 1.00 28 70
	ATOM		005 CE				12.06	3/ 11.000
_	MOTA						13.08	34 11.930 -1.039 1.00 33.42
5	55 ATON			, SE	•		13.03	33 12.850 1.876 1.00 27.92
	OTA	_	007 C	SE:			14.1	76 13.294 1.779 1.00 30.78
	OTA	-	0 800	SE SE		433	12.0	45 13.521 2.459 1.00 28.96
	ATO	-	009 N	<u> </u>		A 433	12.2	69 14.824 3.076 1.00 34.21
	ATO		010 C				_	57 15.387 3.623 1.00 35.07
	60 ATO		011 C					1 00 42 38
	ATO	M 1	012 0	G SE	K .	A 433	10.1	

5	ATOM	1013	С	SER	A	433	13.263	14.644	4.223	1 00	22 42
	ATOM	1014	ō	SER	A	433 [.]	14.152	15.473		1.00	33.43
	ATOM	1015	N	ARG	A	434	13.105	13.545	4.429	1.00	31.94
	ATOM	1016	CA	ARG	A	434				1.00	31.32
	ATOM	1017	CB	ARG	A	434	13.980	13.236	6.086	1.00	29.78
10	ATOM	1018	CG				13.468	11.994	6.819	1.00	29.84
	ATOM	1018	CD	ARG	A	434	14.331	11.541	7.983	1.00	32.17
	ATOM			ARG	A	434	14.626	12.672	8.958	1.00	37.00
		1020	NE	ARG	A	434	15.321		10.140	1.00	39.44
	ATOM	1021	CZ	ARG	A	434	15.935		11.034	1.00	44.06
15	ATOM	1022	NH1	ARG	A	434	15.949		10.885	1.00	45.52
13	MOTA	1023	NH2	ARG	Α	434	16.528		12.084	1.00	45.01
	ATOM	1024	C	ARG	Α	434	15.413	13.014	5.605	1.00	29.24
	MOTA	1025	0	ARG	Α	434	16.352	13.563	6.173	1.00	29.72
	MOTA	1026	N	PHE	Α	435	15.577	12.206	4.561	1.00	28.95
	ATOM	1027	CA	PHE	Α	435	16.901	11.935	4.000	1.00	30.59
20	ATOM	1028	CB	PHE	Α	435	16.777	11.045	2.758	1.00	32.03
	ATOM	1029	CG	PHE	Α	435	16.795	9.563	3.051	1.00	31.88
	MOTA	1030	CD1	PHE	Α	435	16.758	9.084	4.359	1.00	35.60
	ATOM	1031	CD2	PHE	Α	435	16.847	8.643	2.009	1.00	35.89
	ATOM	1032	CE1	PHE	Α	435	16.771	7.709	4.622	1.00	35.36
25	ATOM	1033	CE2	PHE	A	435	16.860	7.271	2.262	1.00	32.71
	ATOM	1034	CZ	PHE	A	435	16.821	6.807	3.570	1.00	33.24
	ATOM	1035	С	PHE	A	435	17.576	13.253	3.607	1.00	
	ATOM	1036	0	PHE	A	435	18.763	13.464			32.73
	ATOM	1037	N	ARG	A	436	16.812	14.137	3.871	1.00	31.16
30	ATOM	1038	CA	ARG	A	436	17.341	15.429	2.975	1.00	33.37
	ATOM	1039	CB	ARG	A	436	16.282		2.549	1.00	39.13
	ATOM	1040	CG	ARG	A	436		16.206	1.756	1.00	40.42
	ATOM	1041	CD	ARG	A	436	16.846	17.317	0.877	1.00	43.09
	ATOM	1042	NE	ARG	A	436	15.750	17.960	0.040	1.00	44.53
35	ATOM	1042	CZ	ARG			14.826	16.955		1.00	48.34
	ATOM	1043	NH1	AŖĢ	A	436	13.530		-0.184	1.00	48.81
	ATOM	1044			Α	436	12.997	17.823	0.619	1.00	47.80
	ATOM	1045	NH2	AŖ <u>G</u>	A	436	12.769	15.950		1.00	49.53
	ATOM		C	ARG	A	436	17.792	16.250	3.753	1.00	38.10
40	ATOM	1047	0	ARG	Ā	436	18.896	16.789	3.764	1.00	41.00
40		1048	N	MET	Α	437	16.936	16.334	4.766	1.00	39.47
	ATOM	1049	CA	MET	A	437	17.257	17.087	5.975	1.00	38.20
	ATOM	1050	CB	MET	A	437	16.102	16.998	6.965	1.00	39.79
•	ATOM	1051	С	MET	Α	437	18.550	16.594	6.626	1.00	41.15
4.5	ATOM	1052	0	MĒŢ	Α	437	19.303	17.378	7.201	1.00	40.20
45	ATOM	1053	N	MET	A	438	18.804	15.285	6.538	1.00	39.65
	MOTA	1054	CA	MET	A	438	20.011	14.693	7.117	1.00	39.70
	MOTA	1055	CB	MET	Α	438	19.787	13.221	7.463	1.00	39.90
	ATOM	1056	CG	MĘŢ	Α	438	18.694	12.938	8.460	1.00	41.94
	MOTA	1057	SD	MET	A	438	18.747	11.188	8.880	1.00	43.12
50	ATOM	1058	CE	MET	Α	438	20.374	11.064	9.619	1.00	43.73
	ATOM	1059	С	MET	Α	438	21.176	14.756	6.142	1.00	38.03
	ATOM	1060	0	MET	Α	438	22.321	14.503	6.522	1.00	
	ATOM	1061	N	ASN	A	439	20.886	15.070			38.39
	ATOM	1062	CA	ASN	A	439	21.924		4.895	1.00	37.64
55	ATOM	1063	CB	ASN	A	439	23.019	15.118	3.895	1.00	35.68
	ATOM	1064	CG	ASN				16.125	4.243	1.00	40.98
	ATOM	1065	OD1	ASN	A A	439	23.933	16.407	3.090	1.00	45.09
	ATOM	1065	ND2			439	23.528	16.295	1.934	1.00	47.16
	ATOM	1067		ASN	A	435	25.197	16.733	3.372	1.00	46.87
60	ATOM		C	ASN	A	439	22.552	13.732	3.739	1.00	31.06
-	ATOM	1068	0	ASN	A	439	23.764	13.581	3.649	1.00	29.54
	AIOM	1069	N	LEU	A	440	21.692	12.698	3.704	1.00	31.47

								11.326	3.579	.00 3	1.63
5	ATOM	1070	CA	LEU		440		10.344	•		3.05
,	ATOM	1071	CB	LEU		440	20.991	8.886			7.07
	ATOM	1072	CG	LEU		440	21.451	8.353			6.18
	ATOM	1073	CD1	LEU	A	440	21.957	8.333			2.33
	ATOM	1074	CD2	LEU	A	440.	20.318				2.10
10	ATOM	1075	С	LEU	A	440	23.146	11.161			2.76
10	ATOM	1076	0	LEU	A	440	22.925	11.671			2.54
	MOTA	1077	N	GLN	A	441	24.225	10.450			1.97
	ATOM	1078	CA	GLN	Α	441	25.255	10.220	2.345		1.75
	ATOM	1079	CB	GLN	A	441	26.632	10.320			5.56
15	ATOM	1080	CG	GLN	Α	441	26.896	11.669	2.979		4.97
13	MOTA	1081	CD	GLN	Α	441	27.040	12.748	1.939		35.51
	MOTA	1082	OE1	GLN	Α	441	27.985	12.782	1.167		35.41
		1083	NE2	GLN	Α	441	26.053	13.659	1.899		34.08
	ATOM	1084		GLN	A	441	25.100	8.860	1.038		30.73
20	MOTA	1085		GLN	A	441	24.540	7.931	1.625		32.78
20	MOTA	1086		GLY	Α	442	25.608	8.752	-0.187	•	32.70
	MOTA	1087		GLY	Α	442	25.528	7.503	-0.921		31.87
	MOTA	1088		GĻY	Α	442	26.181		-0.184		33.18
	ATOM	1089		GLY	A	442	25.642		-0.154		30.60
0.5	MOTA	1090		GLU	Ä	443	27.340	6.603			30.85
25	MOTA	1090		GLU	A	443	28.057	5.567			30.65
	MOTA	1092		GĻŪ	A	443	29.376	6.111			36.30
	MOTA	1093	_	GĽÚ	A	443	30.425	6.378		1.00	40.92
	MOTA	1094		GĻŲ	A	443	30.310	7.770		1.00	40.92
20	MOTA	109		GLU	Α	443	29.677			1.00	46.82
30	MOTA	109			A	443	30.853	8.003		1.00	30.43
	MOTA	109		GLU	A	443	27.206			1.00	28.11
	ATOM	109		GLÜ	A	443	27.211	3.854		1.00	30.26
	ATOM	109		GLU	A	444	26.482	5.95		1.00	28.18
25	MOTA	110		GLU	A	444	25.619			1.00	26.32
35	MOTA	110		GLU	A	444	25.147			1.00	29.27
	MOTA	110		GLU	A	444	26.250			1.00	29.62
	MOTA	110		GĽŪ	A	444	25.748			1.00	32.00
	ATOM	110	_			444	25.006	9.65		100	29.02
40	MOTA	110				444	26.088				26.93
40		110		GLU		444	24.40				24.78
	MOTA	110		GLU		444	23.97				27.79
	ATOM	110		PHE			23.86	1 5.25			24.50
	ATOM	110			_		22.68				25.40
	ATOM	11:					22.25	4 5.41	6 0.610		23.74
45		11:					21.37	2 4.63	4 -0.316	1.00	23.00
	MOTA	11:					20.03	4 4.41	19 -0.004	1.00	22.37
	MOTA	11		=			21.88	5 4.09	4 -1.489	1.00	22.57
	MOTA						19.21		70 -0.85		
	MOTA	11					21.07	9 3.34	49 -2.34	2 1.00	21.69
50		11					19.74	3.1	38 -2.02		
	MOTA			PH			22.91	[3 3.1			
	MOTA		17 C	PH		_	22.08		16 1.79		
	MOTA		18 0	VA		446	24.01		68 0.82		
	MOTA		19 N			446	24.2	78 1.4	81 0.44		
5	5 ATOM		.20 C		-		25.52	22 1.3	60 -0.46	5 1.00	
	ATOM		.21 CI	_		A 446 A 446	25.2		46 -1.79	9 1.00	
	ATOM			G1 VA		A 446	26.7		68 0.21	7 1.00	
	ATOM			G2 VA		A 446	24.4			4 1.00	
	ATOM		L24 C			A 446	24.1				
ϵ	MOTA = 0		125 0			A 447				0 1.00	22.02
	MOTA	1 1:	126 N	CY	. <u></u>	., 11/	22.2				

5	ATOM	1127	CA	CYS-	А	447	25.155	0.503	4.025	1.00	24.17
_	ATOM	1128	CB	CYS	A	447	25.953	1.359	5.011	1.00	23.95
	ATOM	1129	SG	CYS	A	447	27.738	1.324	4.731	1.00	28.57
	ATOM	1130	C	CYS	A	447	23.781	0.178	4.618	1.00	21.14
	ATOM	1131	0	CYS	A	447	23.512	-0.960	5.002	1.00	19.37
10	ATOM	1132	И	LEŲ	A	448	22.915	1.186	4.680	1.00	19.28
	ATOM	1133	CA	LEU	A	448	21.568	1.002	5.219	1.00	21.31
	ATOM	1134	CB	LEU	A	448	20.803	2.324	5.219	1.00	21.31
	ATOM	1135	CG	LEU	A	448	21.142	3.337	6.303	1.00	26.61
	ATOM	1136	CD1	LEU	A	448	20.328	4.594	6.072		27.74
15	ATOM	1137	CD2	LEU	A	448	20.323	2.760		1.00	
13	ATOM	1138	CD2	LEU	A	448	20.827		7.672	1.00	24.03
	ATOM	1138	0	LEU	A	448		-0.038	4.442	1.00	21.72
	ATOM	1140	N	LYS	A	449	20.006 20.929	-0.803	5.030	1.00	20.87
	ATOM	1140	CA					-0.055	3.119	1.00	21.42
20			CB	LYS	A	449	20.205	-0.997	2.269	1.00	20.98
20	ATOM ATOM	1142 1143		LYS	A	449	20.440	-0.659	0.788	1.00	21.55
			CG	LYS	A	449	19.438	-1.297		1.00	24.82
	ATOM ATOM	1144	CD CE	LYS	. A	449	19.456	-0.613		1.00	23.33
		1145 1146		LYS	A	449	20.816	-0.754		1.00	23.58
25	ATOM		NZ	LYS	A	449	20.741	-0.482		1.00	28.77
23	ATOM ATOM	1147	C	LYS	A	449	20.629	-2.436	2.548	1.00	20.33
		1148	0	LYS	A	449	19.800	-3.345	2.552	1.00	20.57
	ATOM	1149	N	SER	A	450	21.924	-2.637	2.777	1.00	19.25
	ATOM	1150	CA	SER	A	450	22.451	-3.965	3.074	1.00	21.84
30	ATOM	1151	CB	SER	A	450	23.982	-3.953	3.041	1.00	20.59
30	ATOM	1152	OG G	SER	A	450	24.460	-3.975	1.702	1.00	29.78
	ATOM ATOM	1153	C	SER	A	450	21.975	-4.408	4.454	1.00	21.58
	ATOM	1154	0	SER	A	450	21.728	-5.590	4.682	1.00	20.06
	ATOM	1155 1156	N CA	ILE	À	451	21.853	-3.449	5.369	1.00	22.20
35	ATOM			ILE	A	451	21.385	3.741	6.726	1.00	22.82
33	ATOM	1157 1158	CB	ILE	A	451	21.452	-2.476	7.616	1.00	19.62
	ATOM	1159	CG2 CG1	ILE ILE	A A	451	20.593	-2.658	8.886	1.00	21.11
	ATOM	1160	CD1	• .		451	22.909	-2.210	7.999	1.00	22.20
	ATOM	1161	CDI	ILÉ	A	451	23.115	-0.960	8.850	1.00	24.48
40	ATOM	1162	0	ILE	A	451	19.952	-4.250	6.662	1.00	21.82
40	ATOM	1163	И	ILE	A	451 452	19.575	-5.184	7.369	1.00	21.72
	ATOM	1164	CA	ILE	A N		19.152	-3.642	5.795	1.00	20.18
	ATOM	1165	CB		A A	452	17.763	-4.058	5.649	1.00	18.13
	ATOM	1166	CG2	IĻE	A	452 452	17.024 15.720	-3.145	4.627	1.00	19.72
45	ATOM	1167	CG1		_	452 452	16.725	-3.792	4.169	1.00	18.99
43	ATOM	1168	CD1	IĻĒ IĻĒ	A	452 452		-1.788	5.282	1.00	18.33
	ATOM	1169	CDI	•	A		16.284	-0.707	4.306	1.00	23.25
	ATOM			IĻĘ	A	452	17.725	-5.517	5.191	1.00	19.50
		1170	0	ILE	A	452	16.980	-6.340	5.737	1.00	17.60
50	ATOM	1171	N	LEU	A	453	18.555	-5.844	4.209	1.00	19.23
50	ATOM	1172	CA	LEÚ	A	453	18.589	-7.205	3.679	1.00	21.60
	ATOM	1173	CB	LEU	A	453	19.624	-7.316	2.554	1.00	21.50
	ATOM	1174	CG	LEU	A	453	19.835	-8.729	1.989	1.00	25.06
	ATOM	1175	CD1	LEU	A	453	18.550	-9.250	1.364	1.00	25.27
55	ATOM	1176	CD2	LEU	A	453	20.948	-8.694	0.953	1.00	24.73
23	ATOM	1177	С	LEU	A	453	18.906	-8.245	4.746	1.00	19.41
	ATOM	1178	0	LEU	Α	453	18.198	-9.241	4.891	1.00	20.75
	ATOM	1179	N	LEU	Α	454	19.966	-7.997	5.499	1.00	21.35
	ATOM	1180	CA	LEU	A	454	20.410	-8.925	6.530	1.00	23.67
60	ATOM	1181	CB	LEU	Α	454	21.870	-8.625	6.878	1.00	20.69
60	ATOM	1182	CG	LEŲ	Α	454	22.816	-8.584	5.673	1.00	24.92
	ATOM	1183	CD1	LEU	Α	454	24.222	-8.268	6.132	1.00	24.27

							22 785 -9.913 4.952 1.00 22.84
5	ATOM	1184	CD2	LEU A		454	22.783
J	MOTA	1185	С	LEU 3		454	19.572
	MOTA	1186	0	LEU .	-	454	19.413
	MOTA	1187	N	ASN		455	19.011 7.681 9.400 1.00 26.10
	ATOM	1188	CA	ASN	A	455	18.439 -6.295 10.002 1.00 22.67
10	ATOM	1189	CB	ASN	A	455	10.439
10	ATOM	1190	CG	ASN	A	455	17.627 -0.100 25 16
	ATOM	1191	OD1	ASN	A	455	
	MOTA	1192	ND2	ASN	A	455	10.013
	MOTA	1193	С	ИЗА	Α	455	10.,00
15	MOTA	1194	0	ASN	A	455	16.230 3.322 8.381 1.00 28.51
13	MOTA	1195	N	SER	Α	456	14 578 -7 704 8.371 1.00 32.52
	MOTA	1196	CA	SER	Α	456	14.3/0 7 022 1 00 35.98
	MOTA	1197	CB	SER	A	456	14.015
	ATOM	1198	OG	SER	Α	456	14.233 -9.086 8.711 1.00 33.00
20	ATOM	1199	С	SER	Α	456	12 112 -9 202 9.523 1.00 33.07
20	MOTA	1200		SER	Α	456	13.112 5.202 8.117 1.00 28.40
	MOTA	1201	N	GLY	A	457	14 115 -11 464 8.413 1.00 36.28
	MOTA	1202	CA	GLY	Α	457	15.055 -12.289 9.277 1.00 40.41
	MOTA	1203	3 C	GLY	A	457	14.831 -13.486 9.456 1.00 38.20
25	ATOM	1204	1 0	GLY	Ά	457	16 005 -11 657 9.820 1.00 44.13
	MOTA	1209	5 N	VAĻ	A	458	17 079 -12 356 10.647 1.00 51.09
	ATOM	120	6 CA	VAL	Α	458	10 214 -11 399 11.095 1.00 51.06
	MOTA	120		VAL	A	458	17 600 -10 390 12.104 1.00 51.75
	MOTA	120		VAĻ	À	458 458	19.365 -12.199 11.692 1.00 50.65
30	MOTA	120		VĄŢ	Ą	458	16 513 -13.060 11.885 1.00 57.26
	MOTA	121		VAĻ	À	458	17.085 -14.045 12.356 1.00 58.77
	MOTA	121		VAL	À	459	15 401 -12.560 12.416 1.00 62.31
	MOTA	121		TYR	A	459	14 793 -13.177 13.592 1.00 68.49
	MOTA	121		TYR	À	459	14 293 -12.100 14.560 1.00 70.46
35	MOTA	121		TÝŘ	A A	459	15 396 -11.196 15.069 1.00 /1./3
	MOTA	121		TYR	Ą A	459	15 127 -9.888 15.462 1.00 /1.93
	MOTA	121			A	459	16 147 -9.045 15.898 1.00 72.80
	MOTA	121				459	16.716 -11.644 15.128 1.00 /2.//
	MOTA	123		*,			17.741 -10.812 13.30
4(12:		TYR			17 450 -9.514 15.941 1.00 72.93
	ATOM	12:		TYR			18 46/ -0.00/ +0.00-
	ATOM	12:		TYR			13.649 -14.097 13.20
	ATOM	12 12		TYR	-		13 380 -15.033 13.034
	MOTA		23 O 24 N	THE			17 981 -13.750
4			25 CA				11 881 -14.30, 44.00
	MOTA		26 CB			460	11.246 -13.300 20.01
	MOTA		27 C	THE		460	12.436 -15.936 11.222 1 00 80 82
	MOTA		28 0	THI		460	11.684 -16.800 10.50-
	MOTA OT		29 N	PH		461	13.762 -10.031 11.00 85 63
3	MOTA 03		230 CA			A 461	14.440 -17.233 10.300
	ATOM		231 CE		•	A 461	15.920 -17.032 10.00 97 52
	ATOM		232 C	PH		A 461	14.284 -10.200 12.00
	ATOM		233 0	PH		A 461	14.493 -17.940 13.222
	ATOM S5 ATOM		234 N	LE	-	A 462	13.914 -19.520 11.72 1 00 91 34
	ATON ATON		235 C			A 462	13.711 -20.500 12.725 1 00 91 23
	ATON		236 CI	=		A 462	12.961 -21.741 12.00
	ATOM		237 C	LE		A 462	15.016 -21.060 13.51
	ATO!	_	238 0	LE		A 462	16.042 -21.103 12.00
	60 ATO		239 N			À 463	14.966 -21.357 14.00
	ATO	_	240 C		ER	A 463	16.131 -21.855 15.358 1.00 92.96
	AIO	-					

_						
5	ATOM	1241 CB	SER;	Α	463	16.033 -21.483 16.833 1.00 91.67
	MOTA	1242 C	SER	Α	463	16.189 -23.371 15.200 1.00 93.39
	MOTA	1243 O	SER	A	463	15.156 -24.034 15.102 1.00 93.44
	MOTA	1244 N	SER	A	464	17.399 -23.917 15.167 1.00 93.82
	MOTA	1245 CA	SER	Α	464	17.577 -25.355 15.015 1.00 93.85
10	ATOM	1246 CB	SER	Α	464	17 004 07 07
	MOTA	1247 C	SER	Α	464	10 005 07 015
	MOTA	1248 O	SER	A	464	
	ATOM	1249 N	THR	Α	465	10 000 00 000 00
	ATOM	1250 CA	THR	A	465	00.500
15	MOTA	1251 CB	THR	A	465	20.600 -26.036 17.212 1.00 93.79
	ATOM	1252 C	THR	À		20.952 -27.483 16.863 1.00 93.38
	ATOM	1253 0	THR		465	21.640 -25.085 16.634 1.00 93.27
	ATOM	1254 N	LEU	A A	465	21.302 -24.017 16.121 1.00 93.03
	ATOM	1255 CA	LEU		466	22.907 -25.479 16.723 1.00 93.26
20	ATOM	1255 CR 1256 CB		A	466	23.999 -24.665 16.207 1.00 92.34
	ATOM	1250 CB	LEU	A	466	25.335 -25.338 16.498 1.00 91.59
	ATOM	1258 0	LEU	A	466	23.829 -24.461 14.706 1.00 92.18
	ATOM	1258 U	LEU	A	466	24.411 -23.545 14.125 1.00 92.67
	ATOM		LYS	A	467	23.028 -25.323 14.086 1.00 91.28
25	ATOM	1260 CA	LYS	A	467	22.772 -25.238 12.653 1.00 90.02
23	ATOM	1261 CB 1262 C	LYS	A	467	21.740 -26.287 12.240 1.00 89.93
	ATOM		LYS	A	467	22.269 -23.841 12.308 1.00 88.35
	ATOM	1263 O	LŸŠ	Α	467	23.032 -22.990 11.849 1.00 88.50
		1264 N	SER	Ä	468	20.981 -23.610 12.536 1.00 86.02
30	ATOM ATOM	1265 CA	SER	A	468	20.384 -22.315 12.252 1.00 84.10
30	ATOM	1266 CB	SER	A	468	18.901 -22.333 12.620 1.00 84.08
	ATOM	1267 OG	SER	A	468	18.229 -23.378 11.937 1.00 83.03
	MOTA	1268 C	SER	À	468	21.109 -21.230 13.040 1.00 83.39
		1269 0	SER	À	468	21.264 -20.105 12.565 1.00 83.48
35	ATOM ATOM	1270 N	LEU	A	469	21.558 -21.579 14.242 1.00 82.04
33		1271 CA	LEÜ	Α	469	22.276 -20.640 15.098 1.00 80.28
	ATOM	1272 CB	ΓĒΩ	Ā	469	22.595 -21.294 16.436 1.00 79.81
	ATOM ATOM	1273 C	LEU	A	469	23.564 -20.174 14.419 1.00 79.18
		1274 0	LEU	A	469	24.111 -19.122 14.756 1.00 78.61
40	ATOM	1275 N	GLÜ	A	470	24.044 -20.969 13.466 1.00 76.69
70	ATOM ATOM	1276 CA	GĽŰ	A	470	25.256 -20.638 12.726 1.00 74.84
		1277 CB	GĻŲ	A	470	25.803 -21.880 12.032 1.00 74.12
	ATOM	1278 C	GLŲ	A	470	24.920 -19.565 11.697 1.00 73.77
	MOTA	1279 0	GLU	A	470	25.617 -18.556 11.581 1.00 72.94
45	ATOM	1280 N	GLU	A	471	23.842 -19.792 10.953 1.00 72.08
73	ATOM	1281 CA	GĽÑ	Α	471	23.396 -18.842 9.945 1.00 70.05
	ATOM	1282 CB	GĨ'n	Α	471	22.461 -19.526 8.944 1.00 71.52
	ATOM	1283 CG	GŢŨ	Α	471	23.150 -19.976 7.668 1.00 72.90
	ATOM	1284 CD	GLÜ	A	471	24.512 -20.586 7.932 1.00 74.01
50	ATOM	1285 OE1	GĽÚ	Α	471	25.469 -20.258 7.198 1.00 74.22
50	ATOM	1286 OE2	GĻŲ	Α	471	24.626 -21.395 8.878 1.00 75.18
	ATOM	1287 C	GĽŬ	A	471	22.667 -17.692 10.630 1.00 67.33
	ATOM	1288 O	GĻŅ	A	471	21.685 -17.165 10.107 1.00 67.77
	ATOM	1289 N	LYS	Α	472	23.152 -17.319 11.811 1.00 62.63
~ ~	ATOM	1290 CA	LYS	Α	472	22.564 -16.229 12.578 1.00 57.41
55	ATOM	1291 CB	LYS	Α	472	21.697 -16.777 13.713 1.00 58.74
	ATOM	1292 CG	LYS	Α	472	20.683 -15.776 14.243 1.00 60.32
	ATOM	1293 CD	LYS	Α	472	19.271 -16.342 14.219 1.00 60.73
	MOTA	1294 CE	LYS	Α	472	18.485 -15.909 15.449 1.00 61.78
	ATOM	1295 NZ	LYS	Α	472	19.352 -15.788 16.658 1.00 60.09
60	ATOM	1296 C	LYS	Α	472	23.662 -15.339 13.150 1.00 53.42
	ATOM	1297 O	LYS	Α	472	23.631 -14.120 12.978 1.00 50.87
						30.87

							24.628 -15.949 13.830 1.00 47.52
5	ATOM	1298 N	1	ASP .	A	473	24.020
_	ATOM	1299 C	A	ASP .	A	473	25.752 25.052
	ATOM	1300 C	В .	ASP .	A	473	20.013
	ATOM	1301 C	G .	ASP	A	473	26.360 13.665
	MOTA	1302 0	D1	ASP	A	473	23.272 23.272 20.00
10	ATOM		D2	ASP	A	473	27.304 20.20 1 00 42 63
	ATOM	1304 C	:	ASP	Α	473	26.337 11.022 20.22
	ATOM	1305 C		ASP	Α	473	27.087
	ATOM	1306 N	J	HIS	Α	474	26.663 -15.364 12.180 1.00 38.05
	ATOM			HIS	Α	474	27.416 -14.904 11.026 1.00 37.25
15	ATOM		CB	HIS	Α	474	27.429 -15.978 9.941 1.00 35.07
13	ATOM	_	CG	HIS	Α	474	28.036 -15.523 8.653 1.00 37.36
	ATOM		CD2	HIS	Α	474	29.292 -15.113 8.355 1.00 38.86
			ND1	HIS	Α	474	27.322 -15.452 7.476 1.00 41.31
	MOTA		CE1	HIS	A	474	28.110 -15.020 6.509 1.00 40.86
20	MOTA		NE2	HIS	A	474	29.311 -14.807 7.016 1.00 44.49
20	MOTA		C	HIS	A	474	26.749 -13.640 10.493 1.00 36.68
	MOTA		0	HIS	A	474	27.417 -12.676 10.132 1.00 36.48
	MOTA			ILE	A	475	25.422 -13.652 10.447 1.00 35.93
	MOTA		N Cr	ILE	A	475	24.683 -12.499 9.963 1.00 36.21
	MOTA		CA		A	475	23.174 -12.797 9.868 1.00 36.31
25	ATOM		CB	IĻĘ	A	475	22.411 -11.527 9.513 1.00 38.19
	MOTA		CG2	ILĖ		475	22.922 -13.874 8.813 1.00 36.97
	MOTA		CG1	ILE	A	475	21.528 -14.454 8.869 1.00 35.59
	MOTA		CD1	ILE	A	475	24.893 -11.322 10.907 1.00 35.34
	MOTA	1322	С	ΙĻĘ	À	475	25.092 -10.189 10.471 1.00 33.20
30	MOTA	1323	0	IĻĒ	A		24.857 -11.596 12.206 1.00 35.95
	MOTA	1324	N	HIS	A	476	25.031 -10.540 13.193 1.00 35.06
	MOTA	1325	CA	HIS	A	476	24.681 -11.062 14.585 1.00 37.30
	MOTA	1326	CB	HIŞ	Α	476	23.210 -11.068 14.860 1.00 43.06
	MOTA	1327	CG	HIŞ	A	476	22.329 -10.051 15.017 1.00 43.93
35	MOTA	1328	CD2	нīй	A	476	22.476 -12.230 14.968 1.00 45.60
	MOTA	1329	ND1	HĮS	À	476	22.470 12.200 17.60
	MOTA	1330	CEl	HIS	Α	476	21.207 22.300 200 46 31
	MOTA	1331	NE2	HIS	A	476	21.091 10.013 10.0 35 40
	ATOM	1332	C	HIS	Α	476	20.430
40	MOTA	1333	0	HIS	À	476	20.034 0.771 201000
	MOTA	1334	N	ARG	À	477	27.420 10.003 22101
	ATOM	1335	CA	ARG	A	477	28.790 10.331 11.04
	MOTA	1336	CB	ARG	Α	477	29.757 -11.500 12.000
	MOTA	1337	CG	ARĢ	A	477	29.000 12.100 =0
45		1338	CD	ARĢ	Α	477	30.762 13.333 20.00
	ATOM	1339	NE	ARG	Α	477	31.760 13.073 21.00
	MOTA	1340	CZ	ARG	À	477	32.700 11.011
	MOTA	1341		ARG	Α	477	32.910 -11.003 13.31
	ATOM	1342		ARG	Α	477	33.643 -12.933 23.100 -1
50		1343		ARG	A	477	28.906 -9.361 11.621 1.00 30.77
50	ATOM	1344		ARG		477	29.462 -8.268 11.753 1.00 33.59
	ATOM	1345		VAL		478	28.369 -9.766 10.475 1.00 27.65
		1346		VAL			28.389 -8.930 9.280 1.00 27.07
	ATOM	1347		VAL			27.658 -9.605 8.100 1.00 28.00
, ,	ATOM						27.672 -8.678 6.890 1.00 25.83
55		1348					28.319 -10.933 7.761 1.00 31.66
	MOTA	1349		VAL			27.689 -7.610 9.584 1.00 26.92
	MOTA	1350					28.216 -6.536 9.294 1.00 26.97
	MOTA	1351		VAL			26 499 -7.702 10.171 1.00 25.74
	MOTA	1352		LEU			25.727 -6.516 10.530 1.00 27.97
60		1353		LEU	*		24.474 -6.912 11.324 1.00 25.55
	MOTA	1354	L CB	LEU	3 P	4/5	

5	ATOM	1355	CG	LEU	70	470	22 211	7 222		
,	ATOM	1356	CD1	LEU	A	479	23.211	-7.229 10.517	1.00	29.01
	ATOM	1357	CD2	LEU	A	479	22.056	-7.503 11.481	1.00	27.05
	ATOM	1358	CD2	•	A	479	22.864	-6.063 9.584	1.00	24.92
		1359		LEU	A	479	26.592	-5.582 11.369	1.00	25.39
10	ATOM		0	LEU	A	479	26.595	-4.370 11.158	1.00	27.39
10	MOTA	1360	N	ASP	A	480	27.324	-6.158 12.320	1.00	26.04
	ATOM	1361	CA	ASP	Α	480	28.206	-5.388 13.193	1.00	27.32
	ATOM	1362	CB	ASP	A	480	28.878	-6.305 14.222	1.00	26.67
	ATOM	1363	CG	ASP	A	480	27.990	-6.602 15.417	1.00	31.02
15	ATOM	1364	OD1	ASP	Α	480	28.355	-7.505 16.198	1.00	31.50
15	ATOM	1365	OD2	ASP	A	480	26.935	-5.944 15.580	1.00	32.21
	ATOM	1366	С	ASP	A	480	29.283	-4.699 12.361	1.00	25.59
	ATOM	1367	0	ASP	Α	480	29.672	-3.562 12.636	1.00	27.15
	ATOM	1.368	N	LYS	A	481	29. 7 67	-5.394 11.340	1.00	25.17
20	ATOM	1369	CA	LYS	Α	481	30.794	-4.830 10.477	1.00	24.93
20	MOTA	1370	CB	LYS	A	481	31.306	-5.890 9.512	1.00	28.42
	ATOM	1371	CG	LYS	A	481	32.158	-6.953 10.188	1.00	35.59
	MOTA	1372	CD	LYS	A	481	32.894	-7.799 9.157	1.00	41.21
	ATOM	1373	CE	LYS	Α	481	33.883	-6.963 8.350	1.00	41.48
25	MOTA	1374	NZ	LYS	Α	481	34.954	-6.388 9.215	1.00	43.22
25	ATOM	1375	С	LYS	A	481	30.260	-3.635 9.696	1.00	26.12
	ATOM	1376	0	LYS	Α	481	30.979	-2.657 9.463	1.00	23.73
	ATOM	1377	N	IĻE	A	482	28. 9 96	-3.705 9.291	1.00	25.44
	MOTA	1378	CA	ΙĻĖ	Ą	482	28.421	-2.598 8.545	1.00	27.69
20	ATOM	1379	CB	ΙĻĘ	А	482	27.066	-2.983 7.915	1.00	27.59
30	MOTA	1380	CG2	IĻĖ	Α	482	26.470	-1.788 7.183	1.00	25.97
	ATOM	1381	CG1	ILE	Α	482	27.274	-4.131 6.922	1.00	23.80
	ATOM	1382	CD1	ILE	Α	482	26.000	-4.838 6.533	1.00	21.30
	ATOM	1383	C	ILE	A	482	28.253	-1.408 9.481	1.00	27.33
25	ATOM	1384	0	IĻĒ	A	482	28.312	-0.256 9.045	1.00	28.55
35	ATOM	1385	N	THR	Α	483	28.046	-1.690 10.768	1.00	25.03
	ATOM	1386	CA	THR	A	483.	27.905	-0.632 11.760	1.00	23.62
	ATOM	1387	CB	THR	Α	483	27.535	-1.192 13.154	1.00	22.18
	ATOM	1388	OG1	THR	A	483	26.181	-1.658 13.133	1.00	25.39
40	ATOM	1389	CG2	THR	A	483	27.673	-0.111 14.226	1.00	25.84
40	ATOM	1390	C	THR	A	483	29.257	0.074 11.858	1.00	23.04
	ATOM	1391	0	THR	A	483	29.331	1.306 11.846	1.00	23.55
	ATOM	1392	N	ASP	A	484	30.324	-0.714 11.960	1.00	22.24
	ATOM	1393	CA	ASP	Ą	484	31.674	-0.152 12.039	1.00	25.48
15	ATOM	1394	CB	ASP	Ā	484	32.718	-1.273 12.107	1.00	26.88
45	ATOM	1395	CG	ASP	Ā	484	32.629	-2.083 13.394	1.00	32.52
	ATOM	1396	OD1	ASP	A	484	32.002	-1.608 14.366	1.00	33.68
	ATOM	1397	OD2	ASP	A	484	33.185	-3.198 13.434	1.00	34.63
	ATOM	1398	C	ASP	Α	484	31.930	0.715 10.807	1.00	25.16
50	ATOM	1399	0	ASP	A	484	32.481	1.812 10.905	1.00	26.05
50	ATOM	1400	N	THR	Α	485	31.505	0.226 9.645	1.00	28.96
	ATOM	1401	CA	THR	Α	485	31.689	0.960 8.394	1.00	26.63
	ATOM	1402	CB	THR	Α	485	31.124	0.166 7.197	1.00	26.12
	ATOM	1403	OG1	THR	A	485	31.753	-1.123 7.132	1.00	24.30
	ATOM	1404	CG2	THR	À	485	31.381	0.907 5.898	1.00	23.31
55	ATOM	1405	C	THR	Α	485	30.994	2.318 8.468	1.00	28.90
	ATOM	1406	0	THR	Α	485	31.583	3.354 8.137	1.00	27.26
	ATOM	1407	N	LĘU	A	486	29.743	2.310 8.915	1.00	24.76
	ATOM	1408	CA	LEU	A	486	28.973	3.537 9.027	1.00	26.19
<i>~</i>	ATOM	1409	CB	LEŲ	Α	486	27.567	3.233 9.547	1.00	27.27
60	ATOM	1410	CG	LEÚ	٠A	486	26.508	2.921 8.486	1.00	23.50
	ATOM	1411	CD1	LEU	A	486	25.210	2.550 9.183	1.00	22.03

MOTA

5	ATOM	1469	CA	GLY	A	494	34.903	14.904 10.873	1.00	41.63
	ATOM	1470	С	GLY	Α	494	33.857	15.060 11.965	1.00	41.18
	ATOM	1471	0	GLY	A	494	33.916	16.011 12.747	1.00	38.22
	ATOM	1472	N	LEU	Α	495	32.905	14.138 12.043	1.00	39.53
	ATOM	1473	CA	LEU	Α	495	31.876	14.248 13.068	1.00	38.91
10	MOTA	1474	CB	LEU	A	495	30.713	13.304 12.769	1.00	39.20
	ATOM	1475	CG	LEU	A	495	29.540	13.901 11.988	1.00	40.73
	ATOM	1475	CD1			495	29.976	14.170 10.553		
				LEU	A				1.00	37.80
	MOTA	1477	CD2	LEU	A	495	28.349	12.943 12.026	1.00	40.94
1.5	MOTA	1478	C	LEU	A	495	32.461	13.923 14.431	1.00	36.01
15	ATOM	1479	0	LEU	Α	495	33.347	13.074 14.544	1.00	34.85
	ATOM	1480	N	THR	Α	496	31.979	14.604 15.459	1.00	37.52
	MOTA	1481	CA	THR	Α	496	32.462	14.350 16.812	1.00	35.45
	ATOM	1482	CB	THR	Α	496	31.925	15.375 17.829	1.00	37.55
	MOTA	1483	OG1	THR	Α	496	30.498	15.263 17.908	1.00	32.93
20	MOTA	1484	CG2	THR	Α	496	32.315	16.797 17.434	1:00	36.16
	MOTA	1485	С	THR	Α	496	31.933	12.987 17.210	1.00	35.67
	MOTA	1486	0	THR	Α	496	31.081	12.427 16.521	1.00	34.34
	ATOM	1487	N	LEU	Α	497	32.429	12.452 18.319	1.00	34.88
	ATOM	1488	CA	LEU	Α	497	31.965	11.151 18.786	1.00	35.67
25	ATOM	1489	CB	LEU	A	497	32.689	10.760 20.074	1.00	41.10
	ATOM	1490	CG	LEU	Α	497	33.714	9.640 19.896	1.00	45.27
	ATOM	1491	CD1	LEU	Á	497	34.755	9.692 21.008	1.00	45.09
	MOTA	1492	CD2	LEU	Α	497	32.988	8.305 19.884	1.00	47.77
	ATOM	1493	C	LEU	Α	497	30.455	11.198 19.026	1.00	33.72
30	ATOM	1494	0	LEU	Α	497	29.712	10.350 18.534	1.00	33.20
	ATOM	1495	N	GLN	A	498	30.006	12.202 19.773	1.00	30.82
	MOTA	1496	CA	GLN	Ä	498	28.586	12.348 20.062	1.00	31.47
	ATOM	1497	CB	GLN	À	498	28.344	13.566 20.951	1.00	30.51
	ATOM	1498	CG	GLN	A	498	26.894	13.796 21.341	1.00	34.38
35	ATOM	1499	CD	GĹN	A	498	26.712	15.130 22.015	1.00	38.60
	ATOM	1500	OE1	GĹŃ	A	498	27.363	16.112 21.686	1.00	42.92
	ATOM	1501	NE2	GLN	A	498	25.809	15.176 23.008	1.00	40.02
	ATOM	1502	C	GLN	A	498	27.776	12.476 18.773	1.00	30.47
	ATOM	1503	Ö	GLN	Α	498	26.682	11.927 18.665	1.00	30.85
40	ATOM	1504	N	GLN	A	499	28.311	13.196 17.793	1.00	29.52
••	ATOM	1505	CA	GLN	A	499	27.603	13.362 16.524	1.00	30.24
	ATOM	1506	CB	GLN	A	499	28.292	14.420 15.661		
	ATOM	1507	CG	GLN	A	499	28.135	15.840 16.191	1.00	30.20
	ATOM			~					1.00	31.60
45		1508	CD	GLN	A	499	28.930	16.849 15.389	1.00	
43	ATOM	1509	OE1	GLN	Α	499	29.956	16.518 14.795	1.00	30.66
	ATOM	1510	NE2	GLN	A	499	28.457	18.089 15.364	1.00	34.17
	ATOM	1511	С	GLN	Α	499	27.529	12.047 15.753	1.00	29.40
	ATOM	1512	0	GLN	Α	499	26.567	11.793 15.032	1.00	30.04
	ATOM	1513	N	ĠĻŅ	Α	500	28.550	11.214 15.903	1.00	25.67
50	MOTA	1514	CA	СĽИ	Α	500	28.577	9.937 15.216	1.00	29.30
	MOTA	1515	CB	GLN	Α	500	29.933	9.276 15.406	1.00	31.52
	MOTA	1516	CG	GĽŅ	A	500	31.012	9.839 14.508	1.00	33.05
	ATOM	1517	CD	GLN	Α	500	32.371	9.370 14.930	1.00	34.84
	ATOM	1518	OE1	GLN	Α	500	32.612	8.194 15.141	1.00	36.47
55	MOTA	1519	NE2	GLŅ	Α	500	33.301	10.324 15.082	1.00	38.25
	MOTA	1520	С	GLŅ	Α	500	27.459	9.017 15.711	1.00	27.98
	ATOM	1521	0	GLN	Α	500	26.700	8.469 14.908	1.00	24.84
	ATOM	1522	N	HIS	Α	501	27.357	8.864 17.029	1.00	26.20
	ATOM	1523	CA	HIS	A	501	26.327	8.021 17.631	1.00	27.63
60	ATOM	1524	СВ	HIS	A	501	26.535	7.919 19.145	1.00	27.97
	ATOM	1525	CG	HIS	A	501	27.892	7.420 19.535	1.00	34.27
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						503	28.726	6.540 18.931	1.00	36.10 °
5	MOTA			HIS	A	501	28.720	7.844 20.676		31.81
	ATOM			HIS	A	501	29.716	7.244 20.758		34.89
	MOTA			HIS	A	501		6.448 19.712		37.46
	MOTA		NE2	HIŞ	A	501	29.854	8.572 17.348		24.93
	MOTA	1530	С	HIS	Α	501	24.935	7.815 17.107		26.73
10	ATOM	1531	0	HIS	Α	501	23.998	9.892 17.379		22.79
	MOTA	1532	N	GLN	A	502	24.796	10.498 17.119		26.14
	MOTA	1533	CA	GLN	Α	502	23.504	12.006 17.371		22.36
	ATOM	1534	CB	GLN	Α	502	23.554		1.00	26.19
	MOTA	1535	CG	GLN	Α	502	23.460	12.378 18.848		28.67
15	MOTA	1536	CD	GLN	Α	502	23.589	13.875 19.089	1.00	28.40
• -	MOTA	1537	OE1	GLN	Α	502	23.632	14.663 18.149		24.72
	ATOM	1538	NE2	GLN	Α	502	23.651	14.268 20.355	1.00	
	ATOM	1539	С	GLN	Α	502	23.056	10.221 15.685	1.00	26.19
	ATOM	1540	0	GLN	Α	502	21.913	9.822 15.453	1.00	24.09
20	ATOM	1541	N	ARG	Α	503	23.955	10.429 14.727	1.00	24.88
20	ATOM	1542	CA	ARG	Α	503	23.630	10.196 13.326	1.00	25.25
	ATOM	1543	CB	ARG	Α	503	24.772	10.668 12.418	1.00	27.63
	ATOM	1544	CG	ARG	Α	503	24.432	10.563 10.932	1.00	28.75
	ATOM	1545	CD	ARG	A	503	25.479	11.222 10.056	1.00	27.72
25	MOTA	1546	NE	ARG	A	503	25.072	11.214 8.654	1.00	29.35
23		1547	CZ	ARG	A	503	24.279	12.126 8.105	1.00	25.84
	ATOM	1548	NH1	ARG	A	503	23.804	13.120 8.840	1.00	27.35
	MOTA	1548	NH2	ARG	A	503	23.962	12.044 6.820	1.00	30.63
	MOTA		C	ARG	A	503	23.347	8.716 13.065	1.00	24.53
20	ATOM	1550		ARG	A	503	22.425	8.375 12.321	1.00	25.90
30	MOTA	1551	0	LEU	A	504	24.143	7.841 13.672	1.00	23.00
	MOTA	1552	N		A	504	23.953	6.406 13.496	1.00	22.60
	MOTA	1553	CA	LEU	A	504	24.971	5.621 14.323	1.00	25.43
	MOTA	1554	CB	1 2 .		504	24.781	4.100 14.344		25.23
	MOTA	1555	CG	LEU	A	504	25.166	3.505 12.991		28.52
35	ATOM	1556	CD1	LEU	A	504	25.627	3.495 15.444		22.14
	MOTA	1557	CD2	ΓĖΩ	A		22.541	6.030 13.934		22.84
	MOTA	1558	С	ΓĒЙ	A	504	21.846	5.288 13.245		21.51
	MOTA	1559	0	LEU	A	504	22.120	6.547 15.083		20.16
	ATOM	1560	N	ALA	A	505	20.784	6.262 15.585		21.08
40	MOTA	1561	CA	AĻĄ	A	505		6.868 16.980		23.57
	MOTA	1562	CB	ALA	A	505	20.605	6.832 14.628		20.20
	MOTA	1563	С	ALA	A	505	19.738	6.164 14.293		17.31
	ATOM	1564	0	ΑŢĄ	Α	505	18.754	8.066 14.184		22.11
	MOTA	1565	N	GĽŃ	Α	506	19.954	8.711 13.277		21.70
45	ATOM	1566	CA	GLN	Α	506	19.013	10.111 12.903		22.26
	ATOM	1567		СЃЍ	A	506	19.502			25.84
	MOTA	1568	CG	GĻŃ	Α	506	19.240	11.158 13.979		32.88
	MOTA	1569	CD	GĽŅ	Α	506	20.187			31.23
	ATOM	1570	OE1	GĻŅ	Α		20.704			
50		1571	NE2	GĽŅ	Α	506	20.423			
•	ATOM	1572		GĻŅ	Α	506	18.813	7.881 12.01		
	ATOM	1573		GLN		506	17.684	7.715 11.55		
	MOTA	1574		LEU		507	19.905	7.354 11.47		
	MOTA	1575		LEU			19.827			
55		1576		LEU			21.231			
33		1577		LEU			22.026			
	ATOM						23.371		3 1.00	27.67
	MOTA	1578					21.264		0 1.00	
	ATOM	1579		LEU			19.090			22.35
	MOTA	1580		LEU			18.242			19.33
60		1583					19.402	·		
	MOTA	1582	S N	ΓĒĹ	J A	308	17.402			

5	ATOM	1583	CA	LEU	A	508	18.755	3.260 11.881	1.00	20.72
	ATOM	1584	CB	LEU	A	508	19.501	2.535 13.001	1.00	22.29
	ATOM	1585	CG	LEU	Α	508	20.977	2.311 12.678	1.00	24.70
	ATOM	1586	CD1	LEU	Α	508	21.642	1.551 13.814	1.00	21.37
	ATOM	1587	CD2	LEU	Α	508	21.095	1.542 11.367	1.00	27.88
10	ATOM	1588	С	LEU	Α	508	17.279	3.396 12.239	1.00	19.14
••	ATOM	1589	0	LEU	Α	508	16.498	2.478 12.003	1.00	17.80
	ATOM	1590	N	LEU	A	509	16.895	4.530 12.815	1.00	19.23
	ATOM	1591	CA	LEU	A	509	15.495	4.747 13.173	1.00	20.14
	ATOM	1592	CB	LEU	A	509	15.347	6.030 13.999	1.00	20.28
15	ATOM	1593	CG	LEU	A	509	15.710	5.858 15.479	1.00	21.35
13		1594	CD1	LEU	A	509	15.354	7.106 16.263	1.00	19.29
	ATOM		CD2	LEU	A	509	14.989	4.656 16.038	1.00	20.84
	ATOM	1595					14.681	4.841 11.885	1.00	21.69
	MOTA	1596	С	LEU	A	509		4.514 11.854	1.00	22.40
••	ATOM	1597	0	ΓΕΛ	A	509	13.493			
20	ATOM	1598	N	ILE	A	510	15.343	5.270 10.815	1.00	20.22
	ATOM	1599	CA	ILE	A	510	14.710	5.397 9.508	1.00	20.40
	ATOM	1600	CB	IĻĒ	A	510	15.720	5.946 8.464	1.00	28.34
	ATOM	1601	CG2	ILE	A	510	15.208	5.710 7.056	1.00	32.54
	ATOM	1602	CG1	ILE	A	510	15.965	7.438 8.696	1.00	28.23
25	ATOM	1603	CD1	ΙĻΕ	A	510	14.789	8.189 9.288	1.00	33.16
	MOTA	1604	С	IĻĒ	Α	510	14.210	4.025 9.049	1.00	23.21
	MOTA	1605	0	ILĒ	Α	510	13.120	3.906 8.474	1.00	21.16
	MOTA	1606	N	LEŲ	Α	511	14.998	2.989 9.323	1.00	18.38
	MOTA	1607	CA	LEU	Α	511	14.633	1.634 8.917	1.00	20.10
30	ATOM	1608	CB	ΓËÜ	A	511	15.754	0.656 9.267	1.00	21.69
	MOTA	1609	CG	ΓEΩ	À	511	17.128	1.022 8.692	1.00	26.03
	ATOM	1610	CD1	LEU	Ą	511	18.024	-0.206 8.724	1.00	22.68
	MOTA	1611	CD2	ΓĖΩ	Α	511	16.996	1.544 7.267	1.00	26.00
	ATOM	1612	С	ΓĒЙ	À	511	13.326	1.181 9.543	1.00	18.51
35	MOTA	1613	0	LEU	Α	511	12.663	0.283 9.025	1.00	17.40
	ATOM	1614	N	SER	Α	512	12.963	1.799 10.664	1.00	18.68
	MOTA	1615	CA	SER	Α	512	11.718	1.471 11.331	1.00	18.67
	MOTA	1616	CB	SER	A	512	11.661	2.117 12.720	1.00	18.58
	ATOM	1617	OG	SER	Α	512	10.315	2.229 13.165	1.00	27.92
40	ATOM	1618	С	SER	Α	512	10.572	1.994 10.464		18.43
	MOTA	1619	0	SER	Α	512	9.584	1.296 10.236	1.00	13.91
	MOTA	1620	N	HIS	A	513	10.713	3.228 9.982	1.00	18.95
	ATOM	1621	CA	HIS	A	513	9.698	3.831 9.124	1.00	20.82
	ATOM	1622	CB	HIS	A	513	10.013	5.315 8.894	1.00	24.36
45	ATOM	1623	CG	HIS	A	513	9.923	6.146 10.136		32.13
	MOTA	1624	CD2	HIS	Α	513	8.863	6.744 10.734	1.00	35.29
	ATOM	1625	ND1	HIS	Α	513	11.010	6.391 10.949	1.00	35.00
	ATOM	1626	CE1	HIS	Α	513	10.624	7.101 11.995	1.00	34.67
	MOTA	1627		HIS	À	513	9.326	7.328 11.889	1.00	35.82
50	ATOM	1628		HIS	À	513	9.650	3.079 7.790	1.00	19.08
•	ATOM	1629		HIS	Α	513	8.575	2.863 7.220	1.00	21.20
	ATOM	1630		ILE	A	514	10.809	2.662 7.297		15.58
	ATOM	1631		ILE	A	514	10.849	1.921 6.038		16.48
	ATOM	1632		ΙĻĒ	A	514	12.312	1.678 5.576		
55	ATOM	1633		ILE	A	514	12.349	0.602 4.499		
55		1634		ILE	A	514	12.891	2.986 5.019		
	ATOM			ILE	A	514	14.393	2.992 4.874		
	ATOM	1635				514	10.112	0.590 6.210		
	ATOM	1636		ILE	A	514	9.364	0.164 5.328		
۲0	ATOM	1637		ARG	A	514	10.301	-0.071 7.347		
60	ATOM	1638		ARG	A A	515	9.585	-1.327 7.564		
	MOTA	1639	CA	D/M	A	213	2.505	1.527 7.504		

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5	ATOM	1640	CB	ARG'	Α	515	9.984	-1.980	8.889	1.00	18.36 °
	MOTA	1641	CG	ARG	A	515	9.173	-3.237	9.213	1.00	17.84
	MOTA	1642	CD	ARG	A	515	9.823	-4.470	8.606	1.00	17.94
	ATOM	1643	NE	ARG.	A	515	11.038	-4.813	9.334	1.00	26.96
	ATOM	1644	CZ	ARG	Α	515	11.406	-6.051	9.641	1.00	25.13
10	MOTA	1645	NHl	ARG	Α	515	10.654	-7.080	9.281	1.00	23.49
	MOTA	1646	NH2	ARG	Α	515	12.511	-6.254		1.00	32.16
	MOTA	1647	С	ARG	Α	515	8.089	-1.020	7.594	1.00	18.29
	MOTA	1648	0	ARG	Α	515	7.275	-1.759	7.038	1.00	16.22
	ATOM	1649	N	HIS	Α	516	7.726	0.085	8.237	1.00	19.33
15	ATOM	1650	CA	HIS	Α	516	6.317	0.441	8.330	1.00	17.78
	MOTA	1651	CB	HIS	Α	516	6.126	1.702	9.166	1.00	16.84
	MOTA	1652	CG	HIS	Α	516	4.692	2.101	9.312	1.00	18.16
	ATOM	1653	CD2	HIS	Α	516	3.967	3.061	8.691	1.00	21.17
	ATOM	1654	ND1	HIS	Α	516	3.830		10.180	1.00	20.70
20	ATOM	1655	CE1	HIS	A	516	2.633		10.089	1.00	21.52
	ATOM	1656	NE2	HIS	Α	516	2.689	2.992	9.191	1.00	20.16
	ATOM	1657	С	HIS	Α	516	5.708	0.659	6.954	1.00	16.63
	ATOM	1658	0	HIŞ	Α	516	4.598	0.216	6.689	1.00	18.58
	ATOM	1659	N	MET	Α	517	6.438	1.334	6.073	1.00	15.29
25	ATOM	1660		MEŢ	Α	517	5.925	1.589	4.730	1.00	16.58
	MOTA	1661		MEŢ	A	51 7	6.837	2.576	4.002	1.00	18.66
	ATOM	1662		MET	Α	517	6.805	3.978	4.631	1.00	16.88
	ATOM	1663		MET	Α	517	7.670	5.243	3.701	1.00	24.08
	MOTA	1664	CE	MET	Ä	517	9.390	4.777	3.962	1.00	14.30
30	ATOM	1665		MET	Α	517	5.773	0.289	3.940	1.00	17.86
	ATOM	1666		MET	A	517	4.791	0.101	3.224	1.00	18.25
	MOTA	1667		SER	Α	518	6.741	-0.610	4.086	1.00	17.43
	MOTA	1668	CA	SER	A	518	6.697	-1.896	3.403	1.00	18.40
	ATOM	1669	CB	SER	Α	518	7.974	-2.695	3.680	1.00	16.77
35	MOTA	1670	OG	SER	Α	518	7.834	-4.030	3.227	1.00	24.23
	ATOM	1671	. С	SER	Α	518	5.476	-2.695	3.854	1.00	17.91
	MOTA	1672	2 0	SER	Ά	518	4.788	-3.295		1.00	18.97
	MOTA	1673	N	ASN	A	519	5.204	-2.697		1.00	21.82
	ATOM	1674	L CA	ASN	Α	519	4.047	-3.418		1.00	21.99
40	ATOM	1675	CB	ASN	Α	519	3.957	-3.257		1.00	23.24
	ATOM	1676	G CG	ASN	A	519	5.046	-4.011		1.00	31.14
	MOTA	1677	OD1	ASN	A	519	5.585	-4.999		1.00	32.50
	MOTA	1678	ND2	ASN	Α	519	5.368	-3.545		1.00	29.10
	ATOM	1679	9 C	ASN	A	519	2.761	-2.871		1.00	23.76
45	MOTA	1680	0 0	ASN	Α	519	1.902	-3.632		1.00	24.48
	MOTA	1683	l N	LYS	Α	520	2.627			1.00	
	MOTA	1682	2 CA	ΓÄĈ	Α	520	1.449			1.00	
	MOTA	1683	3 CB	LYS	Α	520	1.484			1.00	
	MOTA	168	4 CG	LYS	Α	520	1.512			1.00	
50	ATOM	168	5 CD	LYS	Α	520	0.656			1.00	
	MOTA	168	6 CE	LYS	Α	520	-0.787			1.00	
	MOTA	168	7 NZ	LYS	A	520	-1.560				
	MOTA	168	8 C	LYS	Α	520	1.380	-1.144		1.00	
	ATOM	168	9 0	LYS	Α	520	0.316	-1.436			
55	ATOM	169		GLY	Α		2.520	-1.02			
	ATOM		1 CA	GLY	Α		2.561				
	ATOM	169		GLY			2.177				
	ATOM	169		GLY			1.426		3 -0.413		
	ATOM	169		MET			2.696		1.290		
60	ATOM	169		MET			2.393				
50	ATOM		6 CB	MET			3.170		3 2.042	1.00	25.74

5	ATOM	1697	CG	MET	A	522	3.396	-7.308	1.559	1.00	31.06
	ATOM	1698	SD	MET	Α	522	4.572			1.00	34.06
	ATOM	1699	CE	MET	A	522	6.125				29.28
	ATOM	1700	С	MET	Α	522	0.893			1.00	
	ATOM	1701	0	MET	Α	522	0.268			1.00	
10	ATOM	1702	N	GLU	A	523	0.321				25.47
	ATOM	1703		GLU	A	523	-1.110			1.00	24.95
	MOTA	1704		GLU	A	523	-1.555			1.00	27.15
	MOTA	1705		GLU	A	523	-0.830			1.00	31.08
	ATOM	1706		GLU	A	523	-1.153			1.00	38.93
15	ATOM	1707		GLU	A	523		-3.585		1.00	46.90
	ATOM	1708		GLU	A	523	-2.225			1.00	47.40
	ATOM	1709		GLU			-0.337			1.00	47.39
	ATOM	1710		GLU	A	523	-1.872	-4.368		1.00	26.10
	ATOM	1711			A	523	-2.817			1.00	24.25
20	ATOM	1711		HIS	A	524	-1.449			1.00	24.74
20	ATOM		CA	HIS	A	524	-2.093		-0.173	1.00	26.17
		1713	CB	HIS	A	524	-1.481		-0.379	1.00	24.64
	ATOM	1714	CG	HIS	A	524	-2.233		-1.355	1.00	30.59
	ATOM	1715	CD2	HIS	Α	524	-3.227		-1.172	1.00	32.15
25	ATOM	1716	ND1	HIS	Α	524	-2.008		-2.713	1.00	27.46
23	ATOM	1717	CE1	HĮS	Α	524	-2.829	0.502	-3.326	1.00	34.58
	ATOM	1718	NE2	HIS	A	524	-3.580		-2.413	1.00	30.50
	ATOM	1719	С	HIS	Ą	524	-1.996	-3.294	-1.474	1.00	28.06
	ATOM	1720	0	HIS	Α	524	-2.976	-3.419	-2.217	1.00	29.81
20	ATOM	1721	N	ΓĒЙ	A	525	-0.811	-3.824	-1.746	1.00	27.07
30	ATOM	1722	CA	LEU	À	525	-0.594	-4.601	-2.955	1.00	29.30
	ATOM	1723	CB	LEU	A	525	0.865	-5.039	-3.051	1.00	26.39
	ATOM	1724	CG	ΓΕÜ	À	525	1.307	-5.765	-4.321	1.00	29.34
	ATOM	1725	CD1	ΓĒЙ	Ä	525	0.734	-5.076	-5.562	1.00	29.61
2.5	MOTA	1726	CD2	ΓΈΛ	A	525	2.829	~5.769		1.00	29.22
35	ATOM	1727	С	ĽĖŨ	A	525	-1.497	-5.822	-2.950	1.00	31.67
	ATOM	1728	0	LEU	À	525	-2.128	-6.133		1.00	32.45
	MOTA	1729	N	TYR	Α	526	-1.559	-6.512		1.00	36.14
	ATOM	1730	CA	TYR	Ą	526	-2.397	-7.698		1.00	40.36
	ATOM	1731	CB	TYR	A	526	-2.221	-8.350		1.00	45.27
40	ATOM	1732	CG	TYR	Α	526	-2.849	-9.722		1.00	50.62
	MOTA	1733	CD1	TYR	Α	526	-2.114	-10.867		1.00	54.55
	ATOM	1734	CE1	TYR	Α	526	-2.698	-12.136		1.00	57.27
	MOTA	1735	CD2	TYR	A	526	-4.188	-9.876	0.142	1.00	53.48
	ATOM	1736	CE2	TYR	À	526		-11.141		1.00	
45	MOTA	1737	CZ	TYR	A	526		-12.264		1.00	56.60
	ATOM	1738	OH	TYR	A	526		-13.515		1.00	60.70
	MOTA	1739	С	TYR	A	526	-3.852	-7.298			
	ATOM	1740	0	TYR	A	526	-4.673	-8.094		1.00	42.83
	ATOM	1741	N	SER	A	527	-4.158	-6.055		1.00	43.49
50	ATOM	1742	CA	SER	Ą	527	-5.503			1.00	41.55
	ATOM	1743	CB	SER	A	527		-5.523		1.00	44.04
	ATOM	1744	OG	SER	À	527	-5.606	-4.169		1.00	43.47
	ATOM	1745	C	SER	À		-6.954	-3.789		1.00	47.51
	ATOM	1746	0			527	-5.817	-5.356		1.00	44.18
55	ATOM	1747	N	SER	A	527 520	-6.883	-5.757		1.00	44.88
	ATOM	1748		MEŢ	A	528	-4.883	-4.755		1.00	41.79
	ATOM	1748	CA	MEŢ	A	528	-5.047	-4.536		1.00	44.04
			CB	MET	A	528	-3.898	-3.679		1.00	44.78
	ATOM	1750	CG	MET	A	528	-3.965	-2.206		1.00	45.37
60	ATOM	1751	SD	MET	A	528	-5.652	-1.598		1.00	51.83
00	ATOM	1752	CE	MET	A	528	-5.553	-0.004		1.00	46.61
	ATOM	1753	С	MET	Α	528	-5.087	-5.871	-6.071	1.00	44.29

					-5.689 -5.979 -7.137 1.00 44.02 °
5	MOTA	1754 0	MET A	528	-4.443 -6.883 -5.499 1.00 46.78
	ATOM	1755 N	LYS A	529	-4.413 -8.213 -6.099 1.00 51.28
	ATOM	1756 CA	LYS A	529	-3.550 -9.158 -5.261 1.00 50.87
	ATOM	1757 CB	LYS A	529	-2.798 -10.204 -6.071 1.00 50.55
	ATOM	1758 CG	rae y	529	2 549 -11 520 -6.104 1.00 51.25
10	ATOM	1759 CD	LYS A	529	2 616 -12 694 -5.856 1.00 53.22
10	ATOM	1760 CE	LYS A	529	
	ATOM	1761 NZ	LYS A	529	-2.420 -12.53
	MOTA	1762 C	LYS A	529	-5.829 50.700 51.50
	MOTA	1763 0	LYS A	529	-6.325 -3.003 1.00 56 71
15	MOTA	1764 N	CYS A	530	-6.472 -6.301 3100 58 35
13	ATOM	1765 CA	CYS A	530	-7.833 -9.410 1.502 1.00 59 78
		1766 CB	CYS A	530	-8.333 -9.500 2.000 1 00 63.19
	MOTA	1767 SG	CYS A	530	-7.289 -10.304 2.330 a.m. 59.36
	MOTA	1768 C	CYS A	530	-8.766
20	MOTA	1769 0	CYS A	530	-9.644 -9.100 0.02-1 00 59.24
20	MOTA	1770 N	LYS A	531	-8.569 -7.293 5.000 -1 00 60 14
	MOTA	1771 CA	LYS A	531	-9.390 -0.411 01.00
	MOTA	1771 CR	LYS A	531	-9.158 -4.952 0.527 - 0.0 61 48
	MOTA	1772 CB	LYS A	531	-9.073
	MOTA	1774 0	LYS A	531	-9.618
25	MOTA	- ·	ASN A	532	-8.1/9
	MOTA		ASN A		-7.783 -7.050 200 200 62 29
	MOTA	_	ASN A		-8.966 -0.310 100 64 66
	MOTA		ASN A		-8.750 -9.703 20. 0.1-
	MOTA	_		_	-8.344 -10.332 11.332 1 20 63 68
30	MOTA	_			-9.016 -10.030 3.00 59 75
	MOTA	- : :	ASN A		-7.247 -6.710-10.010
	MOTA		ASN A		-7 48 / -0.013 11:000 -
	MOTA	1782 O		533	-6.507 -3.022 3.334 -
	MOTA	1783 N	• • • •	533	-5,954 -4,650 10.000
35		1784 CA		A 533	-6.223 -3.374 3.000
	MOTA	1785 CB	*	A 533	-6.181 -2.103 To., 00
	MOTA	1786 CG	- •••;	A 533	-7.5/4 -3.40/ 2.2.
	MOTA	1787 CG		A 533	-4.452 -4.707 2022
	MOTA	1788 C	•	A 533	-1.846 -3.0/4
40		1789 O		A 534	-1.852 -5.005 -0.10-
	MOTA	1790 N	*	A 534	-2.417 -6.063-10.621 1.00 54.11 -2.67 -6.632 -9.341 1.00 54.02
	MOTA	1791 CA		A 534	-1.767 -0.032 3.0
	MOTA	1792 CE		A 534	-0.300 -6.930 9.001 -
	MOTA	1793 CC	-	A 534	-1.900 -5.635 -8.200 1.00 55.70
4.5		1794 C	با¥VA پVAL	A 534	-2.089 -7.008-11.770 1.00 54.31
	MOTA	1795 C		A 534	-2.519 -8.164-11.780 1.00 51.66
	MOTA	1796 0	VAL	A 535	-1.315 -6.527-12.755 1.00 53.54
	MOTA	1797 N	PRO	A 535	-0.749 -5.172-12.874 1.00 54.28
	MOTA				-0.949 -7.373-13.893 1.00 53.24
5	MOTA 0				0.011 -6.500-14.697 1.00 52.71
	MOTA	1800 C			-0.353 -5.102-14.319 1.00 53.19
	ATOM		G PRO		0 296 -8.664-13.411 1.00 54.25
	ATOM		_	A 535	0 121 -8.768-12.254 1.00 54.56
	ATOM			A 535	-0.203 -9.645-14.299 1.00 53.63
5	55 ATOM			A 536	0 382 -10 926-13 937 1.00 53.11
-	MOTA	1 1805 0	A LEU	A 536	0.250 -12.046-14.763 1.00 51.88
	ATON		B LEU	A 536	0 686 -13 256-13 938 1.00 51.83
	ATON		G LEU	A 536	1 953 -12 917-13.173 1.00 49.51
	ATO		CD1 LEU	A 536	14 449-14 854 1.00 53.43
	60 ATO		CD2 LEU	A 536	10.905 10.000-14.081 1.00 52.58
,	ATO	•	C LEU	A 536	1.093 - 10.000
	1.20.				

5	ATOM	1811	0	LEU	Α	536	2.414	-11.501-15.075	1 00	FF 33
	ATOM	1812	N	TYR	A	537	2.414	-10.462-13.087	1.00	55.33
	ATOM	1813	CA	TYR	A	537	4.057			48.72
	ATOM	1814	CB	TYR	A	537	4.627	-10.501-13.093	1.00	44.22
	ATOM	1815	CG	TYR	A	537		-9.134-12.709	1.00	44.52
10	ATOM	1816	CD1	TYR		537	4.331	-8.053-13.731	1.00	45.18
10	ATOM	1817	CE1		A		3.623	-6.905-13.376	1.00	43.77
	ATOM	1818	CD2	TYR	A	537	3.334	-5.915-14.317	1.00	45.23
	ATOM	1819	CE2	TYR	A	537	4.747	-8.187-15.058	1.00	46.91
	ATOM	1820	CZ	TYR	A	537	4.462	-7.202-16.008	1.00	43.93
15	ATOM	1821	OH	TYR	A	537	3.757	-6.071-15.631	1.00	46.70
13				TYR	A	537	3.472	-5.097-16.565	1.00	48.35
	MOTA MOTA	1822 1823	С О	TYR	A	537	4.401	-11.562-12.056	1.00	41.29
				TYR	A	537	4.330	-11.319-10.856	1.00	41.82
	ATOM	1824	N	ASP	A	538	4.748	-12.748-12.540	1.00	40.34
20	ATOM	1825	CA	ASP	A	538	5.055	-13.896-11.691	1.00	38.84
20	ATOM	1826	CB	ASP	A	538	5.594	-15.037-12.554	1.00	43.47
	ATOM	1827	CG	ASP	A	538	4.571	-15.531-13.566	1.00	47.67
	ATOM	1828	OD1	AŞP	A	538	4.931	-16.373-14.416	1.00	49.33
	ATOM	1829	OD2	ASP	A	538	3.405	-15.073-13.511	1.00	48.07
25	ATOM	1830	C	ASP	A	538	5.991	-13.676-10.508	1.00	37.28
23	ATOM	1831	0	ASP	A	538	5.620	-13.964 -9.371	1.00	38.55
	ATOM	1832	N	LEU	Α	539	7.196	-13.200-10.766	1.00	33.83
	ATOM ATOM	1833	CA	ΓĔЙ	À	539	8.155	-12.959 -9.692	1.00	32.80
		1834	CB	LĘŲ	A	539	9.419	-12.323-10.263	1.00	32.78
30	ATOM	1835	CG	rÉn	A	539	10.561	-12.031 -9.292	1.00	30.93
30	ATOM	1836	CD1	LEU	A	539	10.913	-13.280 -8.492	1.00	33.81
	ATOM	1837	CD2	LEU	A	539	11.758	-11.538-10.077	1.00	25.92
	ATOM ATOM	1838	C	ĻĘŲ	A	539	7.558	-12.050 -8.614	1.00	31.85
		1839	0	LEU	A	539	7.590	-12.367 -7.423	1.00	25.63
35	MOTA MOTA	1840 1841	N	ΓĒΩ	A	540	7.011	-10.917 -9.042	1.00	32.07
33	ATOM		CA	ΓĔΩ	A	540	6.411	-9.976 -8.111	1.00	31.03
		1842	CB	LEU	À	540	5.792	-8.800 -8.861	1.00	30.56
	ATOM	1843	CG	LEU	A	540	5.124	-7.774 -7.945	1.00	31.12
	ATOM ATOM	1844	CD1	LEU	A	540	6.092	-7.357 -6.838	1.00	29.76
40	ATOM	1845 1846	CD2 C	LEU	A	540	4.693	-6.572 -8.762	1.00	30.85
40	ATOM			ΤĔÑ	A	540	5.337	-10.660 -7.282	1.00	34.55
	ATOM	1847 1848	N	ΓĖЙ	A	540	5.316	-10.522 -6.063	1.00	31.60
	ATOM			LEU	A	541	4.446	-11.388 -7.941	1.00	35.64
	ATOM	1849	CA	LEU	A	541	3.378	-12.101 -7.245	1.00	37.84
45		1850	CB	LEU	A	541	2.452	-12.771 -8.255	1.00	38.49
73	ATOM ATOM	1851	CG	LEU	Ā	541		-11.932 -8.678	1.00	39.80
	ATOM	1852	CD1	rën	A	541		-11.476 -7.448	1.00	40.02
		1853	CD2	LEU	A	541	1.713	-10.733 -9.485	1.00	40.48
	ATOM	1854	C	LEU	A	541	3.937	-13.147 -6.275	1.00	40.10
50	MOTA	1855	0	LEU	A	541	3.472	-13.254 -5.137	1.00	42.72
50	ATOM	1856	N	GĽÜ	A	542		-13.915 -6.723	1.00	38.45
	ATOM	1857	CA	GĽÜ	À	542		-14.932 -5.868	1.00	39.59
	ATOM	1858	CB	GĻŲ	A	542		-15.566 -6.564	1.00	41.73
	ATOM	1859	CG	GĻŪ	A	542		-16.327 -7.831	1.00	48.34
55	ATOM	1860	CD	GLÜ	A	542	6.931	-17.747 -7.819	1.00	52.57
55	ATOM	1861	OE1	GĻU	Α	542	8.049	-17.961 -7.298	1.00	52.70
	ATOM	1862	OE2	GĻŲ	Α	542	6.230	-18.647 -8.331	1.00	53.69
	ATOM	1863	C	GĻŪ	Α	542		-14.299 -4.553	1.00	39.94
	ATOM	1864	0	GLU	Α	542	5.567		1.00	40.99
60	ATOM	1865	N	MET	Α	543	6.844	-13.287 -4.663	1.00	38.29
60	ATOM	1866	CA	MET	Α	543	7.380	-12.580 -3.503	1.00	38.11
	ATOM	1867	CB	MĘŢ	A	543	8.242	-11.408 -3.963	1.00	37.34

							9.311 -11.797 -4.953 1.00 40.59
5	ATOM	1868	CG	MET	A	543	9.311
3	ATOM	1869	SD	MET	A	543	10.829 -12.223
	ATOM	1870	CE	MET	A	543	12.014 11.555 2.501 1 00 37 94
	ATOM	1871	С	MET	A	543	6.287 12.001
	MOTA	1872	0	MEŢ	A	543	6.413 -12.127 -1 00 39 44
10	ATOM	1873	N	LEU	A	544	5.216 -11.311 -1.00 1.00 1.00 1.00
10		1874	CA	LEU	A	544	4.100 -11.013 - 1.00 39 88
	MOTA	1875	СВ	LEU	A	544	3.087 -10.344 3.00 42 70
	MOTA	1876	CG	LEU	A	544	1.775
	MOTA MOTA	1877	CD1	LEU	Α	544	2.060 -8.000 2.000 38 47
1.5		1878	CD2	LEU	A	544	0.854 -9.317 3.112 -1 00 42 83
15	MOTA	1879		LEU	A	544	
	MOTA MOTA	1880		LEU	A	544	2.957 -11.000 1 200 16 32
		1881		ASP	A	545	3.367 -13.313 -2.431 -1 00 50 65
	MOTA	1882		ASP	A	545	2.746 -14.430 - 704 1 00 53 67
20	ATOM	1883		ASP	A	545	2.606 -13.017 2.55
20	MOTA	1884		ASP	A	545	1.703 -13.270 3.00 -0.0 -0.0
	MOTA	1889		ASP	Α	545	0.697 -14.500 5.270
	MOTA	1886		ASP	Α	545	1.999 -15.710 1.00 50 74
	ATOM	188		ASP	A	545	3.559 -14.696 -0.527 -1.00 49.39
	MOTA	188		ASP	Α	545	3.004 -13.303 3.00 51 82
25	MOTA	188		AĻĄ	Ą	546	4.8/4 -14.725 0.00-
	ATOM	189		ALA		546	5.750 213.033 01.00
	ATOM	189		AŢĀ		546	7.180 -14.676 0.333 -1 00 54.67
	ATOM	189		ALA	,	546	5.269 -14.424 2100 1 00 52.32
20	MOTA	189	_	ALA	•	546	5.476 -14.940 3.003 1.00 56.66
30		189	-	HIS		547	4.622 -13.270 1.030 -1 00 59.19
	ATOM	189	_	HIS		547	4.102 -12.320 2.56 70
	MOTA	189	_	HIS		547	4.144 -11.017 2.001 1.00 54 64
	MOTA	189		HIS		547	5.489 -10.334 2.00 3.00 53.92
2.5	MOTA	18:				547	6.644 -10.500 2.22 2.00 52 17
35		18:		- T		547	5.748 -9.514 3.523 1.00 52.16
	MOTA	19					7.004 -9.111 3.033 1 00 51 90
	MOTA	19			• •	547	7.570 = 9.696 2.625 = 1.00 62 77
	ATOM	19	_	нį́			2.668 -12.540 5.707 1.00 63.24
4	MOTA	19		HI		547	1.842 -12.120 - 122 2 00 68 37
4			04 N	AR	-	₄ 548	2.381 -14.224 3.200
	MOTA MOTA		05 CA	ĀĀ	iG 2	A 548	1.053 -14.730 3.222 1 00 73 73
			06 CE		ig i	A 548	0.243
	MOTA .		07 CC	- 27	rG i	A 548	-1.149 -14.245 2.20
4			08 CI	_		A 548	-1.081 -12.720 2121
4	MOTA 6.		909 NI		RG	A 548	-2.305 -12.100 -1.00 75.59
	ATOM		910 C		RG	A 548	-2.478 -10.000 3.222
	MOTA		-		RG	A 548	10.464 3.662 1.00 76.00
	MOTA				RG	A 548	-3.627 -10.101 4 061 1.00 74.94
			913 C	_	ŖĢ	A 548	1.179 10.133
	_		914 0	_	RG	A 548	0.19/ -18.05/ 21010
	ATOM		915 N	_	EU	A 549	2.398 -16.665 4.665
	ATOM				EU	A 545	2.669 -17.969 4.055 1.00 77 55
	MOTA		-		EU	A 54	2.9/1 -18.300 3.00 79 13
	ATON	-	.918	_	ΈÜ	A 54	9 3.846 -17.870 5.015 1.00 80.40
	55 ATO		.919		EU	A 54	9 4.892 -17.317 3.213 210 79 46
	ATO				LEU	A 54	9 3.708 -18.341 0.702 1.00 21 38
	ATO				DES	A 60	0 5.390 -3.001 0.235
	HET.				DES	A 60	0 5.834 -1.969 -3.131 -1.00 21 32
	HET				DES	A 60	0 5.038 -0.714 -5.250 - 0.00 25.87
	• -				DES	A 60	0 864 -5 052 1.00
	HET	MTA	1963		=		

5	HETATM	1925	CP1	DES	A	600	2.987	-0.978 -3.784	1.00	23.92
	HETATM	1926	CP2	DES	A	600	1.597	-1.150 -3.684	1.00	29.77
	HETATM	1927	CP3	DES	Α	600	0.842	-1.214 -4.871	1.00	31.40
	HETATM	1928	OP3	DES	Α	600	-0.506	-1.419 -4.824	1.00	33.36
	HETATM	1929	CP4	DES	Α	600	1.421	-1.099 -6.143	1.00	27.01
10	HETATM	1930	CP5	DES	Α	600	2.793	-0.929 -6.230	1.00	27.40
	HETATM	1931	C7	DES	Α	600	5.671	0.461 -5.482	1.00	22.39
	HETATM	1932	C6	DES	Α	600	7.113	0.561 -5.809	1.00	21.75
	HETATM	1933	C5	DES	Α	600	7.541	0.306 -7.131	1.00	19.97
	HETATM	1934	C4	DES	Α	600	8.889	0.429 -7.477	1.00	23.81
15	HETATM	1935	C3	DES	Α	600	9.814	0.804 -6.488	1.00	21.88
	HETATM	1936	О3	DES	Α	600	11.125	0.901 -6.839	1.00	22.32
	HETATM	1937	C2	DES	Α	600	9.423	1.066 -5.161	1.00	19.74
	HETATM	1938	Cl	DES	Α	600	8.066	0.937 -4.838	1.00	21.25
	HETATM	1939	C8	DES	Α	600	4.894	1.765 -5.443	1.00	21.47
20	HETATM	1940	C9	DES	Α	600	4.959	2.468 -4.070	1.00	21.38
	HETATM	1941	CL	CL	Α	601	14.781	-3.035-17.739	1.00	24.10
	ATOM	1942	CB	SER	В	305	12.321	21.086 25.295	1.00	64.27
	ATOM	1943	С	SER	В	305	12.672	22.102 27.548	1.00	64.37
	MOTA	1944	0	SER	В	305	13.701	22.760 27.702	1.00	66.90
25	ATOM	1945	N	SER	В	305	12.045	23.521 25.606	1.00	63.72
	ATOM	1946	CA	SER	В	305	11.875	22.187 26.251	1.00	64.21
	ATOM	1947	N	LEU	В	306	12.193	21.293 28.484	1.00	63.09
	ATOM	1948	CA	LEU	В	306	12.884	21.133 29.757	1.00	60.98
	ATOM	1949	CB	LEU	В	306	11.884	21.200 30.913	1.00	61.23
30	ATOM	1950	CG	LEU	В	306	12.221	20.417 32.183	1.00	62.23
	ATOM	1951	CD1	LEU	В	306	13.304	21.144 32.966	1.00	62.56
	MOTA	1952	CD2	LEU	В	306	10.965	20.258 33.027	1.00	64.31
	MOTA	1953	С	LEU	В	306	13.660	19.819 29.803	1.00	58.39
	MOTA	1954	0	LEU	В	306	14.570	19.654 30.614	1.00	58.56
35	MOTA	1955	N	ALA	В	307	13.293	18.881 28.933	1.00	54.82
	MOTA	1956	CA	ALA	В	307	13.971	17.589 28.861	1.00	50.62
	MOTA	1957	CB	ALA	В	307	13.092	16.584 28.143	1.00	51.30
	ATOM	1958	C	ALA	В	307	15.303	17.719 28.122	1.00	46.84
	ATOM	1959	0	ALA	В	307	16.196	16.885 28.274	1.00	45.62
40	MOTA	1960	N	LEU	В	308	15.431	18.769 27.320	1.00	43.46
	ATOM	1961	CA	LEU	B	308	16.643	18.983 26.542	1.00	43.01
	ATOM	1962	CB	LEU	В	308	16.413	20.100 25.526	1.00	41.32
	MOTA	1963	CG	LEU	В	308	16.315	19.708 24.051	1.00	43.10
	MOTA	1964		LEU	В	308	15.942	18.239 23.903	1.00	40.51
45	ATOM	1965		LEU	В	308	15.287	20.602 23.375	1.00	39.80
	ATOM	1966	С	LEU	В	308	17.874	19.297 27.385	1.00	42.11
	ATOM	1967		LEU	В	308	19.000	19.102 26.932	1.00	44.34
	ATOM	1968	N	SER	В	309	17.669	19.775 28.608	1.00	40.88
	MOTA	1969		SER	В	309	18.796	20.100 29.475	1.00	42.79
50	ATOM	1970	CB	SER	В	309	18.562	21.447 30.163	1.00	41.25
	ATOM	1971		SER	В	309	17.459	21.379 31.046	1.00	46.67
	ATOM	1972	C	SER	В	309	19.072	19.028 30.529	1.00	42.60
	ATOM	1973	0	SER	В	309	20.053	19.119 31.269	1.00	44.18
	ATOM	1974	N	LEU	В	310	18.217	18.012 30.596	1.00	39.44
55	MOTA	1975	CA	LEU	В	310	18.394	16.936 31.569	1.00	37.62
	ATOM	1976	CB	LEU	В	310	17.205	15.969 31.499	1.00	38.84
	MOTA	1977	CG	LEU	В	310	16.216	15.873 32.668	1.00	42.43
	MOTA	1978	CD1	LEU	В	310	16.040	17.219 33.355	1.00	42.55
	MOTA	1979	CD2	LEU	В	310	14.881	15.380 32.138	1.00	39.69
60	ATOM	1980	С	LEU	В	310	19.691	16.174 31.285	1.00	34.11
	ATOM	1981	0	LEU	В	310	20.111	16.070 30.139	1.00	34.41

				_		20.339	15.662 32.326	1.00 34.04
5	MOTA	1982 N	THR	В	311			1.00 32.34
	MOTA	1983 CA		В	311			1.00 31.75
	ATOM	1984 CB		В	311		14.116 34.420	1.00 36.20
	MOTA	1985 OG		В	311			1.00 31.05
	MOTA	1986 CG		В	311	22.782		1.00 32.37
10	MOTA	1987 C	THR	В	311	21.145	13.117 31.899	1.00 28.16
	MOTA	1988 0	THR	В	311	19.967		1.00 33.23
	ATOM	1989 N	ALA	В	312	22.106		1.00 35.63
	ATOM	1990 CA		В	312	21.811	11.20. 02	1.00 34.00
	MOTA	1991 CE	3 ALA	В	312	23.077		1.00 34.29
15	ATOM	1992 C	ALA	В	312	21.210	9.766 32.089	1.00 33.10
	MOTA	1993 O	ALA	В	312	20.226		1.00 33.90
	MOTA	1994 N	ASP	В	313	21.800		1.00 34.19
	ATOM	1995 C	A ASP	В	313	21.304	10.219 35.788	1.00 42.09
	MOTA	1996 CI	B ASP	В	313	22.258	9.358 35.700	1.00 44.87
20	MOTA	1997 C		В	313	23.494	9.858 36.040	1.00 51.57
	ATOM	1998 O	D1 ASP	В	313	24.586		1.00 46.79
	ATOM	1999 O	D2 ASP	В	313	23.377	8.184 35.290	1.00 31.99
	ATOM	2000 C	ASP	В	313	19.925	10.520 34.971	1.00 32.03
	ATOM	2001 0	ASP	В	313	19.056	9.768 35.426	1.00 32.03
25	ATOM	2002 N	GLN	В	314	19.733	11.819 34.763	1.00 29.73
	MOTA	2003 C	A GLN	В	314	18.458	12.457 35.046	1.00 32.88
	MOTA	2004 C	B GLN	В	314	18.562	13.966 34.832	1.00 36.47
	MOTA	2005 C	G GLN	В	314	18.970	14.732 36.085 16.208 35.815	1.00 36.76
	ATOM	2006 C	D GLN	В	314	19.213		1.00 38.79
30	ATOM	2007 C	E1 GLN	В	314	19.300	16.634 34.664 16.995 36.880	1.00 39.72
3.0	MOTA	2008 N	NE2 GLN	l B	314	19.327	11.873 34.116	1.00 29.11
	MOTA	2009	GLN		314	17.409	11.620 34.522	1.00 28.82
	MOTA	2010	GLN		314	16.274	11.657 32.864	1.00 27.27
	ATOM	2011 N	MEI		315	17.801	11.657 32.804	1.00 30.41
35	ATOM	2012 (CA MET		315	16.900	11.079 31.072	1.00 30.10
	MOTA	2013 (CB MET	г в	315	17.595	10.345 29.421	1.00 38.02
	MOTA	2014 (CG MET	r B	315	16.787	11.220 29.065	1.00 41.12
	MOTA	2015	SD ME	г в	315	15.252	12.835 28.611	1.00 39.32
	MOTA	2016	CE ME		315	15.890	9.665 32.311	1.00 27.99
40	ATOM	2017	C ME			16.490	9.351 32.396	1.00 26.60
	MOTA	2018	O ME'			15.302	0	1.00 27.26
	MOTA	2019	N VA			17.481		1.00 24.54
	MOTA		CA VA			17.229		1.00 26.22
	MOTA	2021	CB VA	_		18.554		1.00 29.81
45	MOTA		CG1 VA			18.272		1.00 29.75
	MOTA	2023	CG2 VA			19.302		
	MOTA	2024	C VA			16.326		
	MOTA	2025	O VA			15.397		
	MOTA	2026	N SE			16.601		
50	MOTA	2027	CA SE			15.799		
	ATOM	2028	CB SE			16.358		
	MOTA	2029	OG SE			17.492		
	MOTA	2030	C SE			14.346		
	MOTA	2031	o si		317	13.434		
5.5		2032	N AI		318	14.135		
	MOTA	2033			B 318	12.786		
	ATOM	2034			B 318	12.850		
	MOTA	2035			B 318	12.03		
	MOTA	2036			B 318	10.90		
6		2037			B 319	12.69		
	MOTA	2038	CA L	EU	B 319	12.09	0 1.102 32.032	<u> </u>

5	MOTA	2039	CB	LEU	В	319	13.050	6.635 31.548	1.00	22.03
	ATOM	2040	CG	LEU	В	319	13.264	7.622 30.394	1.00	20.71
	MOTA	2041	CD1	LEU	В	319	14.146	6.995 29.331	1.00	23.60
	ATOM	2042	CD2	LEU	В	319	11.918	8.020 29.803	1.00	23.82
	ATOM	2043	С	LEU	В	319	11.729	5.926 33.564	1.00	27.26
10	MOTA	2044	0	LEU	В	319	10.615	5.396 33.488	1.00	28.91
	MOTA	2045	N	LEU	В	320	12.656	5.516 34.426	1.00	26.58
	MOTA	2046	CA	LEU	В	320	12.399	4.405 35.334	1.00	26.73
	MOTA	2047	CB	LEU	В	320	13.657	4.075 36.145	1.00	26.87
	MOTA	2048	CG	LEU	В	320	14.846	3.460 35.398	1.00	26.15
15	MOTA	2049	CD1	LEU	В	320	16.053	3.375 36.330	1.00	28.04
	MOTA	2050	CD2	LEU	В	320	14.484	2.076 34.895	1.00	26.96
	ATOM	2051	C	LEU	В	320	11.249	4.722 36.290	1.00	29.19
	ATOM	2052	0	LEU	В	320	10.449	3.849 36.631	1.00	26.66
	MOTA	2053	N	ASP	В	321	11.160	5.976 36.719	1.00	29.72
20	MOTA	2054	CA	ASP	В	321	10.112	6.371 37.647	1.00	31.36
	MOTA	2055	CB	ASP	В	321	10.494	7.683 38.336	1.00	36.60
	MOTA	2056	CG	ASP	В	321	11.407	7.461 39.535	1.00	46.11
	MOTA	2057	OD1	ASP	В	321	10.897	7.058 40.605	1.00	46.64
	MOTA	2058	OD2	ASP	В	321	12.635	7.676 39.402	1.00	45.98
25	MOTA	2059	С	ASP	В	321	8.742	6.494 36.989	1.00	28.29
	MOTA	2060	0	ASP	В	321	7.715	6.432 37.661	1.00	27.19
	MOTA	2061	N	ALA	В	322	8.726	6.650 35.672	1.00	28.34
	MOTA	2062	CA	ALA	В	322	7.469	6.779 34.950	1.00	25.55
	MOTA	2063	CB	ALA	В	322	7.668	7.668 33.728	1.00	24.11
30	MOTA	2064	С	ALA	В	322	6.911	5.420 34.523	1.00	22.80
	MOTA	2065	0	ALA	В	322	5.810	5.338 33.979	1.00	24.54 20.16
	ATOM	2066	N	GLU	В	323	7.662	4.355 34.781 3.021 34.386	1.00	21.44
	MOTA	2067	CA	GLU	В	323	7.229	1.982 34.938	1.00	23.72
25	ATOM	2068	CB	GLU	В	323	8.196 9.393	1.746 34.024	1.00	23.72
35	ATOM	2069	CG	GLU	В	323	8.988	1.134 32.685	1.00	25.23
	ATOM	2070	CD	GLU	В	323 323	8.852	1.881 31.692	1.00	21.74
	MOTA	2071	OE1 OE2	GLU	В	323	8.809	-0.095 32.624	1.00	25.49
	ATOM	2072	OE∠ C	GLU GLU	B B	323	5.796	2.696 34.810	1.00	22.35
40	ATOM	2073 2074	0	GLU	В	323	5.409	2.926 35.951	1.00	22.34
40	MOTA	2074	N	PRO	В	324	4.986	2.165 33.880	1.00	19.10
	ATOM	2075	CD	PRO	В	324	5.286	1.806 32.483	1.00	19.11
	ATOM ATOM	2070	CA	PRO	В	324	3.607	1.839 34.242	1.00	22.04
	ATOM	2077		PRO	В	324	2.919	1.658 32.893	1.00	21.96
45	ATOM	2079		PRO	В	324	4.015	1.137 32.015	1:00	24.13
73	ATOM	2080	C	PRO	В	324	3.619	0.556 35.060	1.00	23.44
	ATOM	2081		PRO	В	324	4.590	-0.200 35.028	1.00	22.20
	ATOM	2082	N	PRO	В	325	2.540	0.287 35.801	1.00	24.88
	ATOM	2083	CD	PRO	В	325	1.299	1.068 35.945	1.00	26.67
50	ATOM	2084	CA	PRO	В	325	2.520	-0.940 36.603	1.00	25.10
30	MOTA	2085	CB	PRO	В	325	1.394	-0.691 37.595	1.00	27.09
	ATOM	2086	CG	PRO	В	325	0.448	0.205 36.854	1.00	26.87
	ATOM	2087		PRO	В	325	2.270	-2.192 35.776	1.00	25.77
	MOTA	2088		PRO	В	325	1.853	-2.118 34.617	1.00	21.69
55	MOTA	2089		ILE	В	326	2.538	-3.344 36.379	1.00	24.05
))	ATOM	2089		ILE	В	326	2.301	-4.620 35.722	1.00	22.51
	ATOM	2090		ILE	В	326	3.303	-5.688 36.185	1.00	25.81
	ATOM	2091		ILE	В	326	3.011	-7.018 35.481	1.00	23.78
	ATOM	2092		ILE	В	326	4.729	-5.209 35.900	1.00	25.75
60	ATOM	2093		ILE	В	326	5.241	-5.585 34.533	1.00	
00	ATOM	2094		ILE	В	326	0.893	-5.020 36.149	1.00	23.63
	ATOM	2033	C		נ	220	3.073	2.020 20.21	•	

							0.632 -5.231 37.332 1.00 24.81
5	ATOM	2096 0	I	LE B		326	0.632
,	ATOM	2097 N	I	EU E		327	10.010
	ATOM	2098 CA	I	EU E	3	327	-1.399 3.131
	ATOM	2099 CE	3 I	LEU E	3	327	-2.330 1.127 2.22 1.00 20 69
	ATOM	2100 CC	3 I	LEU E	3	327	-2.201 -3.210 31.00 1 00 14 87
10	ATOM		oi I	LEU I	3	327	-3.245 -2.075 55.110
10	MOTA		D2 1	LEU I	3	327	-2.384 -2.370 33.112 = -1.00 19.87
	ATOM	2103 C]	LEU 1	В	327	-1.662 -0.520 55.655 - 0.00 20 90
	ATOM	2104 0	:	LEU :	В	327	-0.854 7.722 55.1 00 20 92
	ATOM	2105 N	•	TYR	В	328	-2.803 -7.300 3510-
15	ATOM	2106 C	A '	TYR	В	328	-3.202
15	MOTA		B	TYR	В	328	-3.658
	MOTA		:G	TYR	В	328	-2.515
	MOTA		D1	TYR	В	328	-2.110 -10.050 30.00 1 00 28 10
	MOTA		E1	TYR	В	328	-1.034 -11.000 35.150 -
20	ATOM		D2	TYR	В	328	-1.802 -8.302 33.200 1 00 35 30
20	MOTA		E2	TYR	В	328	-0.716 -0.034 33.320 - 1.00 32 59
	MOTA		cz	TYR	В	328	-0.336
	ATOM		OH	TYR	В	328	0.739 -10.237 -0.320 0.0 22 25
	ATOM		3	TYR	В	328	-4.336
25	MOTA		Э	TYR	В	328	-5.115
23	MOTA		N	SER	В	329	-4.420 -10.100 51.000 1 00 29 39
	MOTA		CA	SER	В	329	-5.480 -10.571 55.10
	MOTA		CB	SER	В	329	-5.002 -11.710 32.00
	MOTA	2120	OG	SER	В	329	-6.091 -12.323 32.422
30	MOTA	2121	C	SER	В	329	-6.625 -11.042 51.010 1 00 32 52
•	MOTA		0	SER	В	329	
	MOTA	2123	N	GLU	В	330	-7.792 -11.203 31101-
	MOTA	2124	CA	GLU	В	330	-0.930 -11.770 1 00 45 63
	MOTA	2125	CB	GLU	В	330	10.134 110.48 62
35	MOTA	2126	С	GLU	В	330	-8.493 -13.093 35.491 1.00 45.52 -7.739 -13.851 34.882 1.00 52.37
	MOTA	2127	0	GLU	В	330	0.052 -13 366 36,707 1.00 51.75
	MOTA	2128	N	TYR	В	331	-8.575 -14.596 37.396 1.00 55.25
	MOTA	2129	CA	TYR	В	331	-8.538 -14.365 38.911 1.00 53.04
	MOTA	2130	CB	TYR	В	331	-9.769 -13.668 39.440 1.00 50.70
40	MOTA	2131	CG	TYR	В	331	-10.880 -14.400 39.856 1.00 47.09
	MOTA	2132	CD1	TYR	В	331	12 035 -13 762 40.292 1.00 46.43
	MOTA	2133	CE1	TYR	В	331	0 942 -12 273 39.478 1.00 47.52
	MOTA	2134	CD2	TYR	В	331	-10.993 -11.625 39.913 1.00 43.98
	MOTA	2135	CE2	TYR	В	331	12 096 -12 376 40 314 1.00 44.33
45	MOTA	2136	CZ	TYR	В	331	-13.239 -11.747 40.715 1.00 45.31
	MOTA	2137	OH	TYR	В		9 528 -15 743 37.075 1.00 60.11
	MOTA	2138	С	TYR	В		10 748 -15 569 37 066 1.00 63.13
	MOTA	2139	0	TYR	В		9 952 -16 913 36 809 1.00 61.60
	MOTA	2140		ASP	В		-9 704 -18 124 36 490 1.00 63 58
50	MOTA (2141		ASP	В		10 637 -17.895 35.298 1.00 65.11
	MOTA	2142	CB	ASP	В		11 723 -18 953 35.200 1.00 65.32
	ATOM	2143		ASP	B		-11.420 -20.136 35.463 1.00 63.69
	MOTA	2144			E		-12.876 -18.602 34.866 1.00 63.61
	MOTA	2145					-8.707 -19.227 36.153 1.00 62.86
5		2146		ASP			-7.853 -19.056 35.287 1.00 62.26
	MOTA	2147		ASP			27.653 15.050 55 833 1.00 63.96
	MOTA			PRO			9 808 -20.690 37.875 1.00 64.24
	ATOM			PRO			- 22 503 36 596 1.00 64.24
	ATOM			PRO		3 3 3 3 3 3	22.305 27 274 1 00 64.70
6	MOTA 0	2151		PRO		3 3 3 3 3 3	-8.013 -22.323 347 1.00 65.00
	ATOM		2 CG	PRO)]	в 333	-9-410 22.072 30

5	ATOM	2153 C	PRO	В	333	-8.180 -22.340 35.351 1.00 63.90
	ATOM	2154 0	PRO	В	333	-7.384 -23.214 35.007 1.00 63.70
	MOTA	2155 N	THR	В	334	-9.303 -22.084 34.683 1.00 63.83
	MOTA	2156 CA	THR	В	334	-9.649 -22.832 33.475 1.00 63.77
	MOTA	2157 CB	THR	В	334	-11.065 -22.477 32.975 1.00 64.63
10	MOTA	2158 OG1	THR	В	334	-11.132 -21.078 32.675 1.00 65.95
-	ATOM	2159 CG2	THR	В	334	-12.102 -22.817 34.036 1.00 65.09
	ATOM	2160 C	THR	В	334	-8.634 -22.499 32.388 1.00 62.62
	ATOM	2161 0	THR	В	334	-8.931 -21.774 31.437 1.00 60.15
	MOTA	2162 N	ARG	В	335	-7.432 -23.043 32.553 1.00 63.14
15	ATOM	2163 CA	ARG	В	335	-6.324 -22.820 31.633 1.00 60.70
	MOTA	2164 CB	ARG	В	335	-5.130 -23.667 32.050 1.00 58.73
	MOTA	2165 C	ARG	В	335	-6.667 -23.086 30.174 1.00 59.71
	MOTA	2166 0	ARG	В	335	-6.302 -22.298 29.298 1.00 62.33
	ATOM	2167 N	PRO	В	336	-7.377 -24.194 29.884 1.00 55.25
20	ATOM	2168 CD	PRO	В	336	-7.938 -25.227 30.769 1.00 53.53
	ATOM	2169 CA	PRO	В	336	-7.698 -24.437 28.471 1.00 50.10
	MOTA	2170 CB	PRO	В	336	-8.399 -25.799 28.476 1.00 49.70
	MOTA	2171 CG	PRO	В	336	-8.164 -26.372 29.844 1.00 50.71
	MOTA	2172 C	PRO	В	336	-8.602 -23.324 27.954 1.00 44.54
25	MOTA	2173 0	PRO	В	336	-9.809 -23.342 28.179 1.00 44.14
	MOTA	2174 N	PHE	В	337	-8.007 -22.350 27.274 1.00 39.18
	MOTA	2175 CA	PHE	В	337	-8.764 -21.223 26.742 1.00 38.25
	MOTA	2176 CB	PHE	В	337	-7.850 -20.003 26.567 1.00 36.98 -7.229 -19.517 27.846 1.00 36.81
	MOTA	2177 CG		В	337	7.225
30	MOTA	2178 CD		В	337	5.040 23.722
	MOTA	2179 CD		В	337	0.025
	MOTA	2180 CE		В	337	3.20
	MOTA	2181 CE		В	337	
	MOTA	2182 CZ		В	337	0.001
35	MOTA	2183 C	PHE	В	337	3.20
	MOTA	2184 0	PHE	В	337	-8.962 -22.399 24.658 1.00 36.26 -10.504 -20.828 25.107 1.00 35.85
	MOTA	2185 N	SER	В	338	-11.198 -20.981 23.836 1.00 34.76
	MOTA	2186 CA		В	338	-12.713 -20.948 24.035 1.00 34.85
	MOTA	2187 CE		В	338	-13.164 -19.621 24.235 1.00 33.53
40	MOTA	2188 00		В	338	-10.761 -19.761 23.037 1.00 34.99
	MOTA	2189 C	SER		338	-10.143 -18.855 23.591 1.00 34.32
	MOTA	2190 0	SER		338 339	-11.075 -19.722 21.750 1.00 33.01
	MOTA	2191 N	GLU		339	-10.682 -18.579 20.950 1.00 33.94
4.5	MOTA	2192 C			339	-11.146 -18.737 19.501 1.00 33.79
45	MOTA	2193 CF			339	-10.758 -17.553 18.623 1.00 39.11
	MOTA	2194 CC			339	-10.865 -17.852 17.137 1.00 43.17
	ATOM	2195 CI			339	-11.990 -17.785 16.600 1.00 45.28
	MOTA	2196 O			339	-9.824 -18.152 16.510 1.00 39.19
50	ATOM	2197 0	GLU GLU		339	-11.265 -17.295 21.531 1.00 34.28
50	ATOM	2198 C			339	-10.575 -16.283 21.631 1.00 33.65
	MOTA	2199 0	GLU		340	-12.535 -17.339 21.920 1.00 31.12
	MOTA	2200 N			340	-13.194 -16.164 22.469 1.00 29.10
	MOTA	2201 C			340	-14.696 -16.412 22.573 1.00 33.84
	MOTA	2202 C			340	-12.639 -15.731 23.826 1.00 28.98
55		2203 C			340	-12.431 -14.541 24.060 1.00 30.48
	ATOM	2204 0				-12.407 -16.691 24.719 1.00 26.60
	MOTA	2205 N			341 341	-11.882 -16.386 26.044 1.00 24.20
	ATOM	2206 C				-11.867 -17.643 26.923 1.00 27.0
	MOTA	2207 C			341	-10.851 -18.541 26.515 1.00 33.8
60		2208 0			341 341	-10.479 -15.793 25.960 1.00 23.9
	MOTA	2209 C	SEF	, B	241	

5	ATOM	2210	0	SER	В	341	-10.171	-14.824 26.651	1.00	21.56
	ATOM	2211	N	MET	В	342	-9.631	-16.368 25.114	1.00	26.83
	ATOM	2212	CA	MET	В	342	-8.271	-15.865 24.954	1.00	27.24
	ATOM	2213	CB	MET	В	342	-7.477	-16.758 24.001	1.00	30.45
	ATOM	2214	CG	MET	В	342	-6.038	-16.300 23.802	1.00	35.35
10	MOTA	2215	SD	MET	В	342	-4.866	-17.667 23.777	1.00	44.57
	MOTA	2216	CE	MET	В	342	-4.034	-17.341 22.244	1.00	41.37
	ATOM	2217	C	MET	В	342	-8.322	-14.448 24.385	1.00	25.31
	ATOM	2218	Ō	MET	В	342	-7.653	-13.541 24.874	1.00	26.67
	ATOM	2219	N	MET	В	343	-9.114	-14.278 23.345	1.00	25.75
15	ATOM	2220	CA	MET	В	343	-9.262	-12.979 22.712	1.00	25.47
	ATOM	2221	CB	MET	В	343	-10.210	-13.088 21.528	1.00	23.51
	MOTA	2222	CG	MET	В	343	-9.540	-13.618 20.273	1.00	28.86
	ATOM	2223	SD	MET	В	343	-8.325	-12.456 19.609	1.00	29.25
			CE		В		-9.344	-11.015 19.371		
20	ATOM	2224		MET		343			1.00	28.74
20	ATOM	2225	C	MET	В	343	-9.798	-11.966 23.712	1.00	25.37
	ATOM	2226	0	MET	В	343	-9.360	-10.810 23.728	1.00	24.98
	ATOM	2227	N	GLY	В	344	-10.739	-12.403 24.536	1.00	23.91
	MOTA	2228	CA	GLY	В	344	-11.320	-11.526 25.536	1.00	22.43
25	MOTA	2229	C	GLY	В	344	-10.313	-11.103 26.592	1.00	22.06
25	ATOM	2230	0	GLY	В	344	-10.262	-9.934 26.982	1.00	20.87
	MOTA	2231	N	LEU	В	345	-9.511	-12.048 27.063	1.00	19.36
	ATOM	2232	CA	LEU	В	345	-8.520	-11.748 28.083	1.00	25.74
	MOTA	2233	CB	LEU	В	345	-7.886	-13.040 28.600	1.00	26.78
20	MOTA	2234	CG	LEU	В	345	-8.794	-14.010 29.362	1.00	30.04
30	ATOM	2235	CD1	LEU	В	345	-8.099	-15.357 29.488	1.00	28.39
	ATOM	2236	CD2	LEU	В	345	-9.122	-13.443 30.736	1.00	29.93
	ATOM	2237	C	LEU	В	345	-7.425	-10.822 27.550	1.00	23.24
	ATOM	2238	0	LEU	В	345	-7.037	-9.865 28.212	1.00	23.43
25	ATOM	2239	N	LEU	В	346	-6.937	-11.108 26.350	1.00	21.92
35	ATOM	2240	CA	LEU	В	346	-5.874	-10.303 25.763	1.00	22.71
	MOTA	2241	CB	LEU	В	346	-5.343	-10.962 24.486	1.00	23.17
	MOTA	2242	CG	LEU	В	346	-4.684	-12.331 24.668	1.00	20.66
	ATOM	2243	CD1	LEU	В	346	-4.303	-12.916 23.309	1.00	18.75
40	ATOM	2244	CD2	LEU	В	346	-3.464	-12.188 25.553	1.00	20.84
40	ATOM	2245	C	LEU	В	346	-6.304	-8.873 25.458	1.00	22.99
	MOTA	2246	0	LEU	В	346	-5.540	-7.935 25.695	1.00	22.07
	ATOM	2247	N	THR	В	347	-7.516	-8.699 24.937	1.00	20.53
	ATOM	2248	CA	THR	В	347	-7.987	-7.357 24.608	1.00	21.89
45	ATOM	2249		THR	В	347	-9.152	-7.388 23.601		
45	ATOM	2250	OG1	THR	В	347	-10.218	-8.190 24.123	1.00	19.65
	ATOM	2251	CG2	THR	В	347	-8.676	-7.955 22.262	1.00	22.01
	ATOM	2252	C	THR	В	347	-8.426	-6.590 25.853	1.00	23.60
	ATOM	2253	0	THR	В	347	-8.358	-5.357 25.883	1.00	20.31
50	ATOM	2254	N	ASN	В	348	-8.884	-7.314 26.874	1.00	22.27
50	ATOM	2255	CA	ASN	В	348	-9.293	-6.667 28.114	1.00	23.99
	ATOM	2256	CB	ASN	В	348	-10.008	-7.642 29.056	1.00	22.32
	ATOM	2257	CG	ASN	В	348	-10.342	-7.022 30.398	1.00	28.26
	ATOM	2258	OD1	ASN	В	348	-9.478	-6.746 31.216	1.00	27.14
	MOTA	2259	ND2	ASN	В	348	-11.647	-6.764 30.625	1.00	27.02
55	ATOM	2260	С	ASN	В	348	-8.035	-6.120 28.798	1.00	19.48
	ATOM	2261	0	ASN	В	348	-8.014	-4.991 29.271	1.00	18.26
	ATOM	2262	N	LEU	В	349	-6.984	-6.931 28.832	1.00	19.07
	MOTA	2263	CA	LEU	В	349	-5.724		1.00	20.37
	ATOM	2264	CB	LEU	В	349	-4.716			18.21
60	ATOM	2265	CG	LEU	В	349	-3.297			18.24
	MOTA	2266	CD1	LEU	В	349	-3.323	-6.904 31.356	1.00	12.44

5	MOTA	2267	CD2	LEU	В	349	-2.370	-8.504 29.672	1.00	21.28
	MOTA	2268	С	LEU	В	349	-5.131	-5.307 28.718	1.00	19.92
	MOTA	2269	0	LEU	В	349	-4.738	-4.322 29.349	1.00	16.56
	MOTA	2270	N	ALA	В	350	-5.067	-5.391 27.391	1.00	16.67
	ATOM	2271	CA	ALA	В	350	-4.529	-4.308 26.578	1.00	17.11
10	ATOM	2272	CB	ALA	В	350	-4.587	-4.690 25.095	1.00	14.15
	MOTA	2273	С	ALA	В	350	-5.272	-2.988 26.805	1.00	17.92
	MOTA	2274	0	ALA	В	350	-4.650	-1.926 26.904	1.00	18.71
	ATOM	2275	N	ASP	В	351	-6.600	-3.053 26.857	1.00	17.51
	ATOM	2276	CA	ASP	В	351	-7.409	-1.856 27.074	1.00	16.57
15	ATOM	2277	CB	ASP	В	351	-8.902	-2.202 27.041	1.00	18.97
	ATOM	2278	CG	ASP	B	351	-9.785	-0.974 26.858	1.00	21.80
	ATOM	2279	OD1	ASP	В	351	-9.660	-0.292 25.824	1.00	
	ATOM	2280	OD2	ASP	В	351	-10.604	-0.682 27.754	1.00	24.62
	ATOM	2281	C	ASP	В	351	-7.064	-1.228 28.415	1.00	22.78
20	ATOM	2282	Ö	ASP	В	351	-6.963	-0.009 28.534		16.81
	ATOM	2283	N	ARG	В	352	-6.894	-2.056 29.438	1.00	15.75
	ATOM	2284	CA	ARG	В	352	-6.552		1.00	13.97
	MOTA	2285	CB	ARG	В	352		-1.509 30.742	1.00	16.09
	ATOM	2286	CG	ARG	В	352	-6.728 -8.189	-2.571 31.833 -2.819 32.189	1.00	15.78
25	MOTA	2287	CD	ARG	В	352			1.00	17.93
	ATOM	2288	NE	ARG	В	352	-8.323 -8.010	-3.882 33.279	1.00	19.84
	ATOM	2289	CZ	ARG	В	352		-5.222 32.785	1.00	21.36
	ATOM	2290	NH1	ARG			-7.187	-6.075 33.387	1.00	21.18
	ATOM	2291	NH2	ARG	B B	352	-6.579	-5.741 34.516	1.00	20.51
30	ATOM	2292	C	ARG	В	352	-6.980	-7.275 32.864	1.00	28.51
50	ATOM	2293	0	ARG	В	352	-5.123	-0.975 30.728	1.00	15.81
	ATOM	2294	Ŋ			352	-4.835	0.057 31.339	1.00	15.61
	ATOM	2295	CA	GTA GTA	В	353	-4.231	-1.665 30.019	1.00	15.45
	ATOM	2296	CB	GLU	В	353	-2.838	-1.228 29.935	1.00	16.59
35	ATOM	2297	CG	GLU	B B	353	-1.990	-2.243 29.168	1.00	14.64
"	ATOM	2298	CD	GLU	B	353	-1.554	-3.456 29.973	1.00	18.23
	ATOM	2299	OE1	GLU	В	353	-0.620	-4.355 29.176	1.00	22.72
	ATOM	2300	OE2	GLU		353	-1.099	-5.078 28.275	1.00	21.94
	ATOM	2301	C C	GĽU	В	353	0.599	-4.324 29.442	1.00	24.41
40	ATOM	2302	0	GLU	В	353	-2.729	0.119 29.219	1.00	15.85
70	ATOM	2302	N		B	353	-1.872	0.939 29.540	1.00	13.76
	ATOM	2303	CA	LEU	В	354	-3.594	0.335 28.235	1.00	12.93
	ATOM	2304	CB	LEU	В	354	-3.556	1.575 27.472	1.00	15.33
	ATOM	2305	CG	LEU	B B	354	-4.616	1.534 26.360	1.00	16.44
45	ATOM	2307		LEU		354	-4.174	0.750 25.112	1.00	17.03
73	ATOM	2307	CD1	LEU	В	354	-5.373	0.509 24.189	1.00	16.70
	ATOM	2308		LEU	В	354	-3.069	1.531 24.384	1.00	14.52
			C	LEU	В	354	-3.747	2.805 28.361	1.00	12.78
	ATOM	2310	0	LEU	В	354	-3.123	3.850 28.141	1.00	14.28
50	ATOM	2311	N	VAL	В	355	-4.600	2.682 29.369	1.00	12.60
30	ATOM	2312	CA	VAL	В	355	-4.844	3.791 30.279	1.00	16.78
	ATOM	2313	CB	VAL	В	355	-5.925	3.429 31.327	1.00	16.84
	ATOM	2314		۷ĄĻ	В	355	-6.070	4.561 32.344	1.00	19.88
	ATOM	2315	CG2	VAL	В	355	-7.254	3.187 30.639	1.00	19.33
<i>c c</i>	ATOM	2316	С	VAL	В	355	-3.533	4.161 30.986	1.00	19.17
55	ATOM	2317	0	VAL	В	355	-3.158	5.328 31.049	1.00	17.30
	ATOM	2318	N	HIS	В	356	-2.826	3.160 31.499	1.00	19.68
	ATOM	2319	CA	HIS	В	356	-1.559	3.418 32.177	1.00	20.64
	ATOM	2320	CB	HIS	В	356	-1.110	2.174 32.945	1.00	21.03
<i>-</i> -	MOTA	2321	CG	HIS	В	356	-2.018	1.818 34.085	1.00	22.88
60	ATOM	2322	CD2	HIS	В	356	-3.128	1.045 34.135	1.00	21.70
	MOTA	2323	ND1	HĮS	В	356	-1.838	2.312 35.358	1.00	19.24

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									1.860 36.145 1.00 18.84
_		2324	CE1	HIS	В	356	-2	.802	1 088 35 426 1.00 17.92
	MOTA MOTA		NE2	HIS	В	356		.598	2 961 31.184 1.00 19.67
	MOTA	2326	С	HIS	В	356	-0	.479	4.614 31.547 1.00 19.61
	MOTA	2327	0	HIS	В	356).424	3 413 29.931 1.00 14.92
	ATOM	2328	N	MET	В	357).428	3.830 28.939 1.00 15.13
10	MOTA	2329	CA	MET	В	357		0.428	3.099 27.604 1.00 13.94
10	MOTA	2330	CB	MET	В	357		1.149	3 631 26.476 1.00 14.71
	ATOM	2331	CG	MET	В	357		0.747	3.014 24.826 1.00 17.75
	ATOM	2332	SD	MET	В	357		0.746	1.222 25.122 1.00 15.21
	MOTA	2333	CE	MET	В	357		0.316	5.334 28.699 1.00 14.94
15	ATOM	2334	С	MET	В	357		1.319	6.031 28.560 1.00 17.02
13	ATOM	2335	0	MET	В	357 358		0.909	5.839 28.659 1.00 18.01
	MOTA	2336	N	ILE	В	358		1.122	7.263 28.423 1.00 19.77
	MOTA	2337	CA	ILE	В	358		2.634	7.577 28.287 1.00 23.11
	ATOM	2338		ILE	В	358		2.879	9.080 28.450 1.00 25.00 7.105 26.913 1.00 24.19
20	MOTA	2339		ILE	В	358		-3.137	7.105 20.500
	MOTA	2340		ILE	В	358		4.600	0.033 23.020
	MOTA	2341		ILE	B B	358		-0.501	8.100 25.550
	MOTA	2342		ILE		358		0.080	9.133 43.233
	MOTA	2343		ILE		359		-0.619	7.831 30.730
25	MOTA	2344		ASN		359		-0.029	0.341 31.52
	MOTA	234		asn Asn		359		-0.480	1.120 33.22
	MOTA	234		ASI ASI		359		-1.831	0.11 33.023
	MOTA	234				359		-2.421	9.069 55.012
	MOTA	234						-2.364	1.543 54.02-
30		234		ASI	•			1.473	8.306 31.037 = 1 00 24.19
	MOTA	235		AS				2.152	9.285 32.145 = 1 00 20.82
	MOTA	235		TR	• •		0	1.995	7.149 31.130
	MOTA	235	_	TR		_	0	3.439	5.965 51.520 6.965 51.520
	MOTA	235 235		TR	77	_	0	3.754	5.524 30.676 1 00 18.21
35		23				3 36	0	5.085	3.303 30.21
	MOTA	23				3 36	0	5.310	5.500 20.561 1 00 13.42
	MOTA	23		_		3 36		6.698	5 392 27 633 1.00 15.52
	MOTA		-	-		в 36		4.475	5 5.332 27.762 1.00 13.34
4	MOTA 0			_	RP :	в 36		6.306	5 078 29 800 1.00 16.05
4	MOTA U		60 NE		RP :		50	7.283	5 5 032 27 288 1.00 16.84
	ATOM		61 C2	22 TI		_	60	7.272 5.04	5 296 26.363 1.00 15.11
	ATOM		62 C2	7 3 T 1	R P	_	60	6.43	= 5 115 26 202 1.00 16·14
	ATOM		63 CI	H2 T	RP	_	60	3.97	9 7.939 30.273 1.00 20.13
4	15 ATON		64 C		RP		60	4.99	8.606 30.497 1.00 17.26
_	ATO		365 O		RP	_	60	3.29	8.012 29.135 1.00 19.34
	ATO		366 N		LA	- T	61	3.70	8.900 28.051 1.00 22.01
	ATO		367 C		ĻĀ		61 61	2.68	8.855 26.921 1.00 15.05
	ATO!		368 C	_	LΑ		61	3.88	33 10.336 28.552 1.00 22.55
	50 ATO	M 2	369 C	_	LΑ		361	4.85	58 11.005 28.210 1.00
	OTA		370 C	_	LA.		362	2.93	32 10.794 29.361 1.00 21.35
	OTA	м 2	371 N	_	YS		362	2.9	66 12.139 29.923 1.00 20.13
	OTA	_			LYS		362	1.7	41 12.363 30.811 1.00 25.15
	ATC	M 2			LYS		362	0.4	26 12.417 30.064 1.00 33.57
	55 ATC)M 2			LYS		362	-0.5	63 13.304 30.805 1.00 36.63
	ATC	om 2			LYS		362	-1.6	20 12.490 31.512 1.00 30.05
	TA				LYS LYS	-	362	-2.8	13.276 31.664 1.00 33.07
	TA				LYS	В	362	4.2	12.379 30.757 1.00 27.75
	AT			_	LYS	В	362	4.6	661 13.51/ 30.522
	60 AT	_		•	ARG	В	363	4.8	305 11.302 31.278 1.00 26.61
	AT	OM	2380	N		-			

5	ATOM	2381	CA	ARG	В	363	5.996	11.414 32.109		27.74
	ATOM	2382	CB	ARG	В	363	5.887	10.457 33.298		28.93
	ATOM	2383	CG	ARG	В	363	4.650	10.704 34.158		36.07
	ATOM	2384	CD	ARG	В	363	4.569	9.745 35.344		42.83
	MOTA	2385	NE	ARG	В	363	4.477	8.344 34.928		49.79
10	MOTA	2386	CZ	ARG	В	363	3.395	7.582 35.080	1.00	51.48
	ATOM	2387	NH1	ARG	В	363	2.300	8.081 35.648	1.00	52.17
	ATOM	2388	NH2	ARG	В	363	3.405	6.316 34.668	1.00	40.24
	MOTA	2389	C	ARG	В	363	7.308	11.190 31.367	1.00	25.80
	MOTA	2390	0	ARG	В	363	8.374	11.183 31.975	1.00	29.36
15	MOTA	2391	N	VAL	В	364	7.231	11.009 30.053	1.00	24.28
	MOTA	2392	CA	VAL	В	364	8.431	10.823 29.248	1.00	21.87
	ATOM	2393	CB	VAL	В	364	8.116	10.048 27.947	1.00	21.84
	MOTA	2394	CG1	VAL	В	364	9.267	10.184 26.968	1.00	15.85
	ATOM	2395	CG2	VAL	В	364	7.860	8.560 28.268	1.00	16.24
20	ATOM	2396	С	VAL	В	364	8.925	12.241 28.923	1.00	28.14
	MOTA	2397	0	VAL	В	364	8.219	13.023 28.285	1.00	24.24
	ATOM	2398	N	PRO	В	365	10.141	12.591 29.379	1.00	28.57
	ATOM	2399	CD	PRO	В	365	11.061	11.726 30.137	7 1.00	30.58
	ATOM	2400	CA	PŖO	В	365	10.719	13.919 29.138		32.16
25	MOTA	2401	CB	PRO	В	365	12.189	13.739 29.50	7 1.00	32.70
	ATOM	2402	CG	PRO	В	365	12.170	12.671 30.549		33.35
	MOTA	2403	С	PRO	В	365	10.546	14.464 27.726		32.22
	MOTA	2404	0	PŖŌ	В	365	11.056	13.897 26.76		37.04
	MOTA	2405	N	GĻŸ	В	366	9.821	15.570 27.609		34.09
30	MOTA	2406	CA	GĽŸ	B	366	9.612	16.182 26.31		32.54
	MOTA	2407	С	GLY	В	366	8.241	15.969 25.70		33.46
	ATOM	2408	0	GLY	В	366	7.791	16.779 24.88		33.73
	MOTA	2409	N	PHE	В	367	7.564	14.895 26.09		31.08
	MOTA	2410	CA	ЬĤЕ	В	367	6.250	14.593 25.543		28.60
35	ATOM	2411	CB	PHE	В	367	5.745	13.244 26.05		25.96
	MOTA	2412	CG	PHE	В	367	4.629	12.671 25.23		22.75
	ATOM	2413	CD1	PHE	В	367	3.313	12.771 25.66		22.62
	MOTA	2414	CD2	PHE	В	367	4.897	12.025 24.03		22.29
40	MOTA	2415	CE1	PHE	В	367	2.272	12.233 24.91		25.63
40	ATOM	2416	CE2	PHE	В	367	3.867	11.486 23.27		20.82
	MOTA	2417	cz	PHE	В	367	2.553	11.588 23.71		25.50
	ATOM	2418	C	PHE	В	367	5.178	15.646 25.78 16.001 24.85		26.79
	ATOM	2419	0	PHE	В	367	4.458 5.049	16.001 24.85		23.37 31.26
A E	ATOM	2420	N	VAL	В	368				35.71
45	ATOM	2421		VAL	В	368	4.020	17.151 27.27 17.412 28.79		35.71
	ATOM	2422	CB	VAL	В	368	3.817			37.64
	ATOM	2423		VAL	В	368	2.944	16.320 29.39		35.81
	ATOM	2424		VAL	В	368	5.157	17.495 29.50		
50	ATOM	2425		VAL	В	368	4.328	18.482 26.59		35.87
50	ATOM	2426	0	VAL	В	368	3.450	19.330 26.45		37.71 35.49
	ATOM	2427		ASP	В	369	5.572	18.665 26.17		
	ATOM	2428		ASP	В	369	5.950	19.904 25.50		36.54
	ATOM	2429		ASP	В	369	7.466	19.963 25.30		39.79
E F	ATOM	2430		ASP	В	369	8.213	20.169 26.61		44.33
55	ATOM	2431		ASP	В	369	9.409	19.807 26.68		48.45
	ATOM	2432		ASP	В	369	7.604	20.693 27.57		43.27
	ATOM	2433		ASP	В	369	5.248	19.997 24.14		34.49
	ATOM	2434		ASP	В	369	5.131	21.074 23.57		34.51
<i>c</i> 0	MOTA	2435		LEU	В	370	4.776	18.859 23.65		30.97
60	ATOM	2436		LEU	В	370	4.086	18.809 22.37		29.80
	ATOM	2437	CB	LEU	В	370	4.145	17.389 21.79	9 1.00	27.27

							5 500	16.733 21.688 1	.00 2	8.07
5	MOTA	2438	CG	LEU E		370	5.522			0.38
•	MOTA	2439	CD1	LEU E	-	370	5.353			2.82
	ATOM	2440	CD2			370	6.316	4 ,		8.04
	ATOM	2441	C	LEU !		370	2.628	T)		9.71
	MOTA	2442	0	LEU 1		370	2.066	19.645 21.425		8.70
10	ATOM	2443	N	THR		371	2.011			0.31
	ATOM	2444	CA	THR	В	371	0.602			1.96
	ATOM		CB	THR	В	371	0.150			9.49
	ATOM		OG1	THR	В	371	0.284			9.98
	ATOM	2447	CG2	THR	В	371	0.991			30.59
15	ATOM	2448	С	THR	В	371	-0.208			27.10
13	ATOM	2449	0	THR	В	371	0.300			27.65
	ATOM	2450	N	LEU	В	372	-1.461	18.863 22.087		30.86
	ATOM	2451	CA	LEU	В	372	-2.323			30.11
	ATOM	2452	CB	LEU	В	372	-3.722	18.147 22.737		32.80
20	ATOM	2453	CG	LEU	В	372	-4.715	17.006 22.960		34.10
20	ATOM	2454	CD1	LEU	В	372	-4.231	16.147 24.126		31.16
	ATOM	2455	CD2	LEU	В	372	-6.105	17.562 23.246		31.77
	ATOM	2456	С	LEU	В	372	-2.437	16.863 21.034	_	27.06
	MOTA	2457	Ō	LEU	В	372	-2.417	15.629 21.078		31.30
25	ATOM	2458	N	HIS	В	373	-2.564	17.548 19.905		31.35
23	ATOM	2459	CA	HIS	В	373	-2.685	16.888 18.614		34.30
	ATOM	2460	CB	HIS	В	373	-2.844	17.935 17.503	1.00	41.27
	ATOM	2461	CG	HIS	В	373	-2.503	17.430 16.132	1.00	42.50
	MOTA	2462	CD2	HIS	В	373	-3.293	17.105 15.079	-	43.69
30	ATOM	2463	ND1	HIS	В	373	-1.205	17.220 15.715	1.00	48.87
30	ATOM	2464		HIS	В	373	-1.210	16.787 14.465	1.00	43.72
	ATOM	2465		HIS	В	373	-2.465	16.708 14.056	1.00	28.29
	MOTA	2466		HIS	В	373	-1.468	16.012 18.337	1.00	30.21
	MOTA	2467		HIS	В	373	-1.610	14.878 17.897	1.00 1.00	28.85
35	ATOM	2468		ASP	В	374	-0.275		1.00	28.28
33	ATOM	2469		ASP	В	374	0.950		1.00	31.33
	ATOM	2470		ASP	В	374	2.178			39.07
	ATOM	2471		ASP	В	374	2.433		1.00	40.60
	MOTA	2472		ASP	В	374	3.195		1.00	38.64
40	MOTA	2473			В	374	1.874		1.00	29.05
40	ATOM	2474		ASP	В	374	1.029			24.26
	ATOM	2475		ASP	В	374	1.432		1.00 1.00	24.52
	ATOM	2476		GLN	В	375	0.642			27.37
	ATOM	247		GĽŅ	В	375	0.667		1.00 1.00	26.66
45		2478		GLN	В	375	0.213		1.00	29.74
7.7	ATOM	247		GLN	В	375	1.164			33.13
	MOTA	248		GLN	В	375	0.623		1.00 1.00	32.82
	ATOM	248			В	375	-0.04			33.98
	MOTA	248			В	375	0.89	5 16.953 25.236	1.00	24.52
50		248		GLN	В	375	-0.25		1.00	23.56
50	ATOM	248		GLN	В	375	0.07	4 11.451 21.221	1.00	21.87
	ATOM	248		VAL		376	-1.42	6 13.013 20.599		23.44
	ATOM	248				376	-2.40	9 12.055 20.140		
	ATOM	248				376	-3.71	8 12.760 19.717		
F		248					-4.57	2 11.823 18.877		
5:		248					-4.48			
	MOTA	248		VAL			-1.85	2 11.257 18.965	1.00	
	MOTA			VAL			-1.94	9 10.032 18.938	3 1.00	
	MOTA			HIS			-1.25	11.953 18.00	7 1.00	
	MOTA	_					-0.68	9 11.284 16.84		
6	MOTA 0						-0.07			25.27
	MOTA	249	94 CB	HTS	, -					

										- 00	20 62
5	ATOM	2495	CG	HIS	В	377	0.535	11.690 1			30.63 31.03
	ATOM	2496	CD2	HIS	В	377	1.828	11.559 1		1.00	35.05
	ATOM	2497	ND1		В	377	-0.217	11.086 1		1.00	33.12
	MOTA	2498	CE1	HIS	В	377	0.588	10.607 1		1.00	31.06
	MOTA	2499	NE2	HIS	В	377	1.833	10.882 1		1.00	24.37
10	ATOM	2500	С	HIS	В	377	0.365	10.237 1		1.00	
	ATOM	2501	0	HIS	В	377	0.321	9.109 1		1.00	21.47
	ATOM	2502	N	LEU	В	378	1.307	10.609		1.00	19.24
	ATOM	2503	CA	LEU	В	378	2.365	9.691		1.00	20.09
	ATOM	2504	CB	LEU	В	378	3.363	10.402		1.00	18.64
15	ATOM	2505	CG	LEU	В	378	4.230	11.489		1.00	22.15
15	ATOM	2506	CD1	LEU	В	378	5.104	12.148		1.00	22.51
	ATOM	2507	CD2	LEU	В	378	5.094	10.885		1.00	20.68
	ATOM	2508	C	LEU	В	378	1.832	8.433		1.00	18.91
	ATOM	2509	0	LEU	В	378	2.262	7.320		1.00	17.52
20	ATOM	2510	N	LEU	В	379	0.888	8.610	20.077	1.00	18.25
20	ATOM	2511	CA	LEU	В	379	0.317		20.795	1.00	18.60
	ATOM	2512	CB	LEU	В	379	-0.526		21.968	1.00	16.77
	MOTA	2513	CG	LEU	В	379	0.292	8.353	23.214	1.00	17.90
	ATOM	2514	CD1	LEU	В	379	-0.578	9.092	24.211	1.00	15.84
25	MOTA	2515	CD2	LĘU	В	379	0.851		23.842	1.00	22.09
23	MOTA	2516	C	LEU	В	379	-0.518	6.605	19.872	1.00	20.17
	ATOM	2517	0	LEU	В	379	-0.476		19.968	1.00	18.11
	ATOM	2518	N	GLU	₿	380	-1.273	7.222	18.971	1.00	19.40
	MOTA	2519		GĻÜ	B	380	-2.086		18.049	1.00	20.19
30	ATOM	2520		GĻŪ	Ρ̈́	380	-2.994	7.350	17.222	1.00	22.43
30	ATOM	2521		GLU	В	380	-4.182		18.007	1.00	25.30
	ATOM	2522		GLU	В	380	-5.070	8.789	17.188	1.00	29.44
	MOTA	2523		GLU	В	380	-6.206		17.625	1.00	31.70
	MOTA	2524		GLU	В	380	-4.631		16.110	1.00	31.75
35	ATOM	2525		GLU	В	380	-1.210		17.117	1.00	18.92
33	ATOM	2526		GLÜ	В	380	-1.586		16.722	1.00	19.83
	MOTA	2527		ACYS		381	-0.039		16.772	0.75	17.41
	MOTA	2528		BCYS		381	-0.035	6.113	16.779	0.25	17.76
	ATOM	2529		ACYS		381	0.860		15.887	0.75	20.19
40	ATOM	2530		BCYS		381	0.875		15.884	0.25	17.50
40	MOTA	2531		ACYS		381	1.870		15.248	0.75	24.20
	ATOM	2532		BCYS		381	1.830	6.406	15.226	0.25	
	ATOM	2533		ACYS		381	1.167		14.060	0.75	
•	ATOM	2534		BCYS		381	3.048		14.128	0.25	
45	ATOM	2535		ACYS		381	1.626		16.592	0.75	
43	ATOM	2536		BCYS		381	1.689		16.561	0.25	
	MOTA	253		ACYS		381	1.737		16.069	0.75	
	ATOM	253		BCYS		381	1.904		15.982		
	ATOM	253		ALA	В	382	2.134		17.785	1.00	
50		254		ALA	В	382	2.955		18.530	1.00	20.27
50				ALA	В	382	4.135		19.143	1.00	18.68
	ATOM	254		ALA	В	382	2.356		19.607		16.82
	MOTA	254		ALA	В	382	3.070		20.142		13.37
	ATOM	254		TRP	В	383	1.074		19.916		
	MOTA	254		TRP	_	383	0.487		21.013		
55		254					-1.009		21.160		
	ATOM	254		TRP	В	383	-1.87		20.129		
	MOTA	254		TRP	В		-2.49		20.198		
	MOTA	254					-3.22		19.003		
	MOTA	254			В				2 21.155		
60		255					-2.50		2 18.933		
	MOTA	255	1 CD1	TRP	В	383	-2.23				

_	2001	2552	NE1	TRP	В	383	-3	.051	1.439	18.250	1.00	23.67
5	ATOM	2552	CZ2	TRP	В	383		.963	-0.853	18.733	1.00	21.55
	ATOM	2554	CZ3	TRP	В	383		.243	-1.702	20.888	1.00	20.29
	ATOM		CH2	TRP	B	383		.960	-1.844		1.00	19.03
	ATOM	2555 2556	Cn2	TRP	В	383		.701	0.579	21.020	1.00	17.35
10	ATOM	2557	0	TRP	В	383		.982	0.010	22.077	1.00	13.92
10	ATOM	2558 2558	И	LEU	В	384		.568	-0.087		1.00	14.07
	MOTA		CA	LEU	В	384		.773	-1.532		1.00	15.98
	ATOM	2559 2560	CB	LEU	В	384		.181	-2.200		1.00	12.19
	ATOM		CG	LEU	В	384		173	-3.735		1.00	12.97
	MOTA	2561	CD1	LEU	В	384		352	-4.240		1.00	10.65
15	ATOM	2562		LEU	В	384).707	-4.259		1.00	17.84
	ATOM	2563	CD2 C	LEU	В	384		2.262	-1.861		1.00	14.64
	MOTA	2564	0	LEU	В	384		2.627	-2.833		1.00	13.78
	MOTA	2565 2566	И	GLU	В	385		3.116	-1.046		1.00	14.96
20	ATOM		CA	GLU	В	385		1.565	-1.260		1.00	13.79
20	MOTA	2567	CB	GLU	В	385		5.336	-0.179		1.00	15.34
	MOTA	2568	CG	GLU	В	385		5.297	-0.312		1.00	15.38
	ATOM	2569 2570	CD	GTA	В	385		6.162		16.520	1.00	23.97
	ATOM		OE1	GLU	В	385		7.381		16.358	1.00	21.03
25	ATOM	2571		GLU	В	385		5.622		16.149	1.00	22.19
25	MOTA	2572 2573		GLU	В	385		4.963		20.987	1.00	15.79
	ATOM	2573 2574		GLU	В	385		5.788		21.463	1.00	15.04
	MOTA	2575		ILE	В	386		4.389		21.690	1.00	13.32
	ATOM	2575 2576		ILE	В	386		4.723	-0.019	23.108	1.00	14.06
20	ATOM ATOM	2576 2577		ILE	В	386		4.173		23.614	1.00	15.36
30	ATOM	2578		ILE	В	386		4.374		25.130	1.00	15.97
	MOTA	2579		ILE	В	386		4.910	2.476	22.907	1.00	17.95
	MOTA	2580		ILE	В	386		4.118		22.874	1.00	21.12
	ATOM	2581		ILE	В	386		4.227		23.993	1.00	14.97
35	ATOM	2582		ILE	В	386		4.905		24.941	1.00	19.60
33	MOTA	2583		LEU	В	387		3.038		23.709	1.00	15.18
	ATOM	2584		LEU	В	387		2.516		24.478	1.00	15.98
	ATOM	2589		LEU	В	387		1.070		24.080	1.00	17.15
	ATOM	2586		LEU	В	387	-	0.031		24.486	1.00	19.65
40	ATOM	258		LEU	В	387	-	-1.371		23.972	1.00	17.77
	ATOM	2588		LEU	В	387	-	-0.075		26.002	1.00	
	ATOM	2589		LEU	В	387		3.391		24.180	1.00	
	ATOM	259		LEU	В	387		3.712		25.076	1.00	
	ATOM	259		MET	В	388		3.785		22.921	1.00	
45	ATOM	259		MET	В	388		4.602		22.547		
	ATOM	259	3 CB	MET	В	388		4.673		21.026	1.00	
	ATOM	259	4 CG	MET	В	388		3.403		20.453		
	MOTA	259	5 SD	MET	В	388		3.364		18.675		
	MOTA	259	6 CE	MET	В	388		1.906		5 18.511		
50	ATOM	259	7 C	MET	В	388		6.004		2 23.133		
	ATOM	259	8 0	MET	В	388		6.460		5 23.636		
	ATOM	259		ILE	В	389		6.707		3 23.074		
	ATOM	260		ILE	В	389		8.044		9 23.634		
	ATOM	260		ILE	Ŗ	389		8.836		1 23.322		
55	ATOM	260			В	389		8.330		6 24.158		
	MOTA	260			В	389		10.325		4 23.602		
	ATOM	260			В	389		11.228		2 23.357		
	ATOM	260		ILE	В	389		7.950		6 25.147		
	ATOM	260		ILE	В			8.844		4 25.739		
60		260		GĻY		390		6.855	-4.00	7 25.761	1.00	
	ATOM	260		GLY		390		6.681	-4.21	9 27.189	1.00	14.87

5	ATOM	2609	С	GLY	В	390	6.444	-F 702 27 462	1 00	30.54
•	ATOM	2610	0	GLY	В	390	6.989		1.00	18.54
	ATOM	2611	N	LEU	B	391			1.00	16.54
	ATOM	2612	CA	LEU	В		5.623		1.00	16.15
	ATOM	2613	CB	LEU		391	5.334		1.00	18.91
10	ATOM	2614	CG		В	391	4.332		1.00	19.55
10	ATOM	2615		LEU	В	391	4.157		1.00	20.91
	ATOM	2616	CD1	LEU	В	391	3.580		1.00	19.41
	ATOM		CD2 C	LEU	В	391	3.232		1.00	20.70
	ATOM	2617	_	LEU	В	391	6.649		1.00	20.31
15		2618	0	LEU	В	391	7.002		1.00	18.66
15	ATOM	2619	N	VAL	В	392	7.378		1.00	18.71
	ATOM	2620	CA	VAL	В	392	8.649		1.00	19.51
	ATOM	2621	CB	VAL	В	392	9.288		1.00	23.77
	ATOM	2622	CG1	VAL	В	392	10.751		1.00	24.63
20	ATOM	2623	CG2	VAL	В	392	8.520	· · · =	1.00	19.94
20	MOTA	2624	С	VAL	В	392	9.615		1.00	22.80
	MOTA	2625	0	LAV	В	392	10.336		1.00	19.36
	MOTA	2626	N	TRP	В	393	9.617	-7.522 27.046	1.00	22.10
	MOTA	2627	CA	TRP	В	393	10.492	-7.241 28.171	1.00	23.20
25	ATOM	2628	CB	TRP	В	393	10.388	-5.773 28.578	1.00	19.22
25	MOTA	2629	CG	TRP	В	393	11.056	-5.479 29.895	1.00	22.53
	MOTA	2630	CD2	TRP	В	393	12.453	-5.591 30.193	1.00	20.36
	MOTA	2631	CE2	TRP	В	393	12.624	-5.208 31.545	1.00	25.65
	ATOM	2632	CE3	TRP	В	393	13.578	-5.976 29.449	1.00	22.12
20	ATOM	2633	CD1	TRP	В	393	10.452	-5.046 31.044	.1.00	23.02
30	MOTA	2634	NE1	TRP	В	393	11.387	-4.881 32.037	1.00	24.91
	ATOM	2635	CZ2	TRP	В	393	13.876	-5.200 32.171	1.00	23.00
	ATOM	2636	CZ3	TRP	В	393	14.829	-5.968 30.072	1.00	23.98
	ATOM	2637	CH2	TRP	В	393	14.964	-5.582 31.423	1.00	23.20
3.5	ATOM	2638	C	TRP	В	393	10.208	-8.114 29.388	1.00	24.36
35	MOTA	2639	0	TRP	В	393	11.128	-8.717 29.944	1.00	23.04
	MOTA	2640	N	ARG	В	394	8.952	-8.189 29.819	1.00	21.29
	MOTA	2641	CA	ARG	В	394	8.680	-9.003 30.990	1.00	22.43
	ATOM	2642	CB	ARG	В	394	7.365	-8.601 31.667	1.00	23.97
40	ATOM	2643	CG	ARG	В	394	6.259	-8.149 30.759	1.00	26.16
40	ATOM	2644	CD	ARĢ	В	394	5.026	-7.727 31.574	1.00	20.86
	ATOM	2645	NE	ARG	В	394	3.817	-7.937 30.786	1.00	19.54
	MOTA	2646	CZ	ARG	В	394	3.327	-7.059 29.915	1.00	20.58
	ATOM	2647	NH1	ARG	В	394	3.944	-5.902 29.722	1.00	17.41
	MOTA	2648	NH2	ARG	В	394	2.229	-7.347 29.220	1.00	16.82
45	MOTA	2649		ARG	В	394	8.695	-10.502 30.713	1.00	21.78
	ATOM	2650	0	ARG	В	394	8.657	-11.294 31.648	1.00	23.44
	ATOM	2651	N	SER	В	395	8.767	-10.880 29.438	1.00	17.10
	ATOM	2652	CA	SER	В	395	8.805	-12.289 29.041	1.00	25.08
	ATOM	2653	CB	SER	В	395	8.206	-12.473 27.638	1.00	19.47
50	ATOM	2654	OG	SER	В	395	6.832	-12.136 27.619	1.00	21.73
	ATOM	2655	С	SER	В	395	10.239	-12.831 29.031	1.00	26.29
	MOTA	2656	0	SER	В	395		-14.030 28.854	1.00	23.75
	ATOM	2657	N	MET	В	396		-11.938 29.210	1.00	30.79
	MOTA	2658	CA	MET	В	396		-12.307 29.205	1.00	35.07
55	ATOM	2659	CB	MET	В	396		-11.063 29.423	1.00	33.84
	ATOM	2660	CG	MET	В	396		-10.569 28.171	1.00	36.88
	ATOM	2661	SD	MET	В	396	15.149		1.00	40.96
	MOTA	2662	CE	MET	В	396	16.675	-9.849 28.998	1.00	39.67
	MOTA	2663	C	MET	В	396		-13.353 30.250	1.00	35.88
60	MOTA	2664	Ō	MET	В	396		-14.215 30.011	1.00	34.52
	ATOM	2665	N	GLU	В	397		-13.266 31.410	1.00	36.19
								200 51.410	1.00	30.13

						12.604 -14.206 32.492 1.00 39.24
5	ATOM	2666 CA	GL.		397	12.604 11.605 22 221 3 00 44 38
	ATOM	2667 CE	GL		397	12.153
	ATOM	2668 CG	GL.	U B	397	606 1 00 56 78
	ATOM	2669 CI		U B	397	13.483 -12.567 55.66
	MOTA	2670 OF		JU B	397	13.380 -11.621 30.470 -100 60 82
10		2671 O	_		397	13.975 -13.666 56.65
10	MOTA	2672 C	GI		397	11.8/8 -15.520 52.275
	MOTA		_	LU B	397	12.021 -10.433 33.14
	MOTA			is B	398	11.100 -13.003 31.20-
	MOTA			IS B	398	[0.34/ -10.025 5000
	MOTA	2675 C			398	8.863 -16.567 31.178 1.00 29.87
15	MOTA	2676 C			398	8.582 -16.111 32.574 1.00 31.80
	MOTA				398	8.215 -16.801 33.678 1.00 29.12
	MOTA				398	8 727 -14.799 32.972 1.00 33.27
	ATOM			IS B	398	2 462 -14 701 34.262 1.00 32.19
	MOTA			IS B		9 149 -15 902 34.714 1.00 33.48
20	MOTA	2681 N		IS B	_	10 556 -17.317 29.492 1.00 25.95
	ATOM	2682		IIS B	_	9.637 -17.291 28.672 1.00 27.47
	MOTA	2683		HIS B		11.771 -17.801 29.186 1.00 29.09
	MOTA	2684 1		PRO B		12 026 -17 922 30 096 1.00 29.93
	MOTA	2685	CD F	PRO B		12.926 -17.922 55 55 6 00 07 40
25	MOTA		CA I	PRO E		12.079
20	ATOM		CB 1	PRO E		13.434 -10.300 20.20.20.20.21
	ATOM		CG 1	PRO E		14.062 -18.201 25.210 1 00 29 76
	MOTA		C	PRO E		11.009 -19.240 27.55
	ATOM			PRO I		10.552 -20.15, 20.55
30	ATOM			GĽÝ I	3 400	10.601 -19.033 20.072 -
30	MOTA				B 400	9.588 -19.664 25.166
	ATOM		-		B 400	8.161 -19.557 25.615 1 00 28 36
		2694			B 400	7.220 -20.155 25.000
	MOTA	2695			B 401	7.996 -16.554 20.725
25	MOTA	2696	-		B 401	6.668 -18.139 27.1200 -1 00 28.50
35	MOTA	2697	CB		B 401	6.435 -16.505 25.6
	MOTA	2698	CG		B 401	6.476 -20.005 20.00
	ATOM	2699	CD	LYS	B 401	6.181 -20.333 30.32
	ATOM	2700	CE	LYS	B 401	6.073 -21.847 30.033 - 00 42 39
	ATOM		NZ	LYS	B 401	7.1// -22.611 23.303 -
40		2701		LYS	B 401	6.493 -10.022 27.000
	ATOM	2702	0	LYS	B 401	7.465 -15.072 27.00-
	MOTA	2703	N	LEU	B 402	5.241 -10.101 20.000
	MOTA	2704			B 402	4.929 -14.735 20.520 -
	MOTA	2705		leŭ Leŭ	B 402	4.088 -14.449 25.689 1.00 10.47
45		2706	CB		B 402	4.798 -14.673 24.360 1.00 10.03
	MOTA	2707	CG	LEU	B 402	3.821 - 14.395 23.211 1.00 21.23
	MOTA	2708	CD1	LEU	B 402	6.011 -13.760 24.277 1.00 23.13
	MOTA	2709		LEU	B 402	4.147 -14.399 28.179 1.00 19.00
	MOTA	2710		LEU		3 024 -14.880 28.381 1.00 18.03
50	MOTA 0	2711		LEU		A 743 -13.559 29.019 1.00 19.54
	MOTA			ΓĖΩ		4 099 -13 148 30.259 1.00 20.21
	ATOM	2713	CA	LEU	B 403	5 155 -12.856 31.332 1.00 23.16
	ATOM		CB	LEU	B 40	$\frac{1}{2}$ -2. (2) 22 766 1 00 29.54
	ATOM		CG	LEU	B 40	3 4.659 -12.662 -1.00 32.67
5	5 ATOM			LEU	B 40	3 5.519 -13.433 33.138 1.00 32.38
,	ATOM			LEU	B 40	3 4.626 -11.213 30 043 1.00 20.42
	ATOM			LEU	B 40	3.219 -11.310 301-1-1 1.00 19.18
	ATOM			LEU	в 40	3.638 -10.787 30.222 1.00 21.44
	MOTA			PHE	B 40	4 2.003 -12.143 29.340 1.00 21.69
4	ATON ATON			PHE	B 40	1.066 -11.055 25.0
•	ATON ATON			PHE	в 40	-0.199 -11.598 28.687 1.00 17.26
	ATO	., 2,2,	-	•		

¥

5	ATOM	2723	·CG	PHE	В	404	-0.026	-11.897 27.227	1.00	19.75
	ATOM	2724	CD1	PHE	В	404	0.364	-13.167 26.801	1.00	17.90
	ATOM	2725		PHE	В	404	-0.210	-10.897 26.280	1.00	17.04
	ATOM	2726	CE1	PHE	В	404	0.572	-13.434 25.447		
	ATOM	2727	CE2	PHE	В	404	-0.007		1.00	19.88
10	ATOM	2728	CZ					-11.148 24.924	1.00	18.47
10				PHE	В	404	0.386	-12.418 24.503	1.00	16.45
	ATOM	2729	C	PHE	В	404	0.768	-10.403 30.685	1.00	21.95
	ATOM	2730	0	PHE	В	404	0.656	-9.177 30.804	1.00	22.99
	ATOM	2731	N	ALA	В	405	0.670	-11.247 31.702	1.00	21.12
	ATOM	2732	CA	ALA	В	405	0.424	-10.814 33.066	1.00	22.43
15	ATOM	2733	CB	ALA	В	405	-1.074	-10.603 33.304	1.00	24.69
	ATOM	2734	C	ALA	В	405	0.959	-11.926 33.962	1.00	22.40
	ATOM	2735	0	ALA	В	405	1.133	-13.061 33.517	1.00	21.67
	MOTA	2736	N	PRO	В	406	1.246	-11.612 35.230	1.00	25.60
	ATOM	2737	CD	PRO	В	406	1.129	-10.294 35.878	1.00	23.65
20	ATOM	2738	CA	PRO	В	406	1.765	-12.632 36.148	1.00	25.91
	ATOM	2739	CB	PRO	В	406	1.899	-11.882 37.475	1.00	27.04
	ATOM	2740	CG	PRO	В	406	2.017	-10.431 37.068	1.00	26.56
	ATOM	2741	С	PRO	В	406	0.876	-13.873 36.259	1.00	
	ATOM	2742	ō	PRO	В	406	1.368	-14.967 36.538		25.12
25	ATOM	2743	N	ASN	В	407	-0.426	-13.713 36.039	1.00	28.92
	ATOM	2744	CA	ASN	В	407	-1.345	-14.852 36.109	1.00	23.53
	ATOM	2745	CB	ASN	В	407	-2.553		1.00	24.09
	ATOM	2746	CG	ASN	В	407		-14.526 36.986	1.00	24.08
	ATOM	2747	OD1	ASN	В		-3.327	-13.328 36.486	1.00	26.72
30	ATOM	2748	ND2	ASN ASN		407	-2.851	-12.574 35.635	1.00	22.65
30	ATOM	2749	C		В	407	-4.528	-13.140 37.019	1.00	26.46
				ASN	B	407	-1.820	-15.231 34.714	1.00	26.91
	ATOM	2750	0	ASN	В	407	-2.859	-15.870 34.548	1.00	28.68
	ATOM	2751	N	LEU	В	408	-1.059	-14.816 33.708	1.00	27.28
25	ATOM	2752	CA	LEU	В	408	-1.387	-15.124 32.327	1.00	27.23
35	ATOM	2753	CB	LEU	В	408	-2.247	-14.030 31.699	1.00	26.61
	MOTA	2754	CG	LEU	В	408	-2.815	-14.464 30.341	1.00	27.51
	ATOM	2755	CD1	LĖU	В	408	-3.702	-15.692 30.546	1.00	28.75
	ATOM	2756	CD2	LEU	В	408	-3.598	-13.330 29.694	1.00	25.48
4.0	ATOM	275 7	С	LEU	В	408	-0.113	-15.316 31.514	1.00	27.56
40	ATOM	2758	0	LEŲ	В	408	0.247	-14.465 30.695	1.00	26.86
	MOTA	2759	N	LEU	В	409	0.553	-16.426 31.759	1.00	27.54
	ATOM	2760	CA	LEU	В	409	1.786	-16.774 31.065	1.00	31.96
	ATOM	2761	CB	LEU	В	409	2.786	-17.355 32.058	1.00	31.88
	ATOM	2762	CG	LEU	В	409	4.186	-17.703 31.562	1.00	37.72
45	ATOM	2763	CD1	LEU	В	409		-16.551 30.770	1.00	39.57
	ATOM	2764	CD2	LEU	В	409	5.066		1.00	41.72
	ATOM	2765	С	LEU	В	409	1.401		1.00	31.53
	ATOM	2766	0	LEU	В	409	0.921		1.00	32.67
	ATOM	2767	N	LEU	В	410	1.604		1.00	29.58
50	ATOM	2768	CA	LEU	В	410	1.228		1.00	31.55
	ATOM	2769	CB	LĘŪ	₽	410	0.192		1.00	29.83
	ATOM	2770	CG	LEU	B	410		-17.080 27.452		
	ATOM	2771	CD1	LEU	В	410		-16.135 26.501	1.00	28.55
	ATOM	2772	CD2	LEU	В	410			1.00	26.92
55	ATOM	2773	CDZ	LEU				-18.200 27.891	1.00	30.49
J J	ATOM	2774			В	410		-18.839 26.814	1.00	33.88
	ATOM	2775	O NT	LEU	В	410		-18.170 26.726	1.00	36.49
			N	ASP	В	411		-20.013 26.206	1.00	38.80
	ATOM	2776	CA	ASP	В	411		-20.562 25.336	1.00	38.39
60	ATOM	2777	CB	ASP	В	411		-21.990 25.752	1.00	44.53
60	ATOM	2778	CG	ASP	₿	411		-22.943 25.749	1.00	44.90
	ATOM	2779	OD1	ASP	В	411	1.773	-23.035 24.719	1.00	45.70

					2.254 -23,603 26.786 1.00 50.54
5	MOTA	2780 OD2	ASP. B	411	20 551 23 909 1.00 38.57
J	ATOM	2781 C	ASP. B	411	1 540 -20 341 23.686 1.00 36.48
	ATOM	2782 0	ASP B	411	2 625 - 20 777 22,949 1.00 36.85
	ATOM	2783 N	ARG B	412	2 259 -20 763 21.541 1.00 38.32
	ATOM	2784 CA	ARG B	412	1 00 38 69
10	ATOM	2785 CB	ARG B	412	700 1 00 40.05
10	ATOM	2786 CG	ARG B	412	10 10 42.98
	ATOM	2787 CD	ARG B	412	5.644 - 22.552 17 636 1 00 40.95
	MOTA	2788 NE	ARG B	412	5.540 -22.55 - 6 752 1 00 41 11
	ATOM	2789 CZ	ARG B	412	4.649 -22.555 10.755 - 1 00 44.01
1.5		2790 NH1	ARG B	412	3.777 -23.430 17.222
15	MOTA	2791 NH2	ARG B	412	4.632 -22.031 13.00 37.64
	ATOM	2792 C	ARG B	412	2.10/ -21./12 22.00 3.6 51
	ATOM	2793 0	ARG B	412	1.28/ -21.42/ 20.000
	ATOM	2794 N	ASN B	413	2.041 -22.834 21.520
	ATOM	2795 CA	ASN B	413	0.974 -23.756 22.000
20	MOTA	2796 CB	ASN B	413	1 1/0 =25.055 22.01
	MOTA	2797 CG	ASN B	413	2.01726.100 21.301 2.00 46 11
	ATOM	2798 OD1		413	2.309 -26.022 20.701 1.00 47.04
	MOTA	2799 ND2		413	7 4 18 -27.104 22.07
	MOTA	2800 C	ASN B	413	-0.383 -23.100 21.502 - 1.00 32 43
25	ATOM	2800 0	ASN B	413	_1 149 -23.372 22.5
	MOTA		GLN B		-() 44 / -22.33 / 23.000
	ATOM		GLN B		-1.685 -21.741 23.
	MOTA		GLN E	_	-1.558 -21.172 24.003 1 00 32 31
	ATOM		GLN E		-1.528 -22.242 25.00 1 00 34 63
30	ATOM		GLN F		-1.293 -21.667 27.527
	MOTA				-0 176 -21.277 27.000
	ATOM			_	
	MOTA	2808 NE		3 414	19 (152 120·030 22·110
	MOTA	2809 C		B 414	-7 195 -20.20 4 22.100
35		2810 0		B 415	-1 ()// -20 130 Z1 00 -
	MOTA	2811 N		B 415	-1.350 -19.180 20.00
	MOTA	2812 CA 2813 C	•	B 415	-2 184 -19.725 15.55
	MOTA			B 415	-2 918 -19.000 10.00
	MOTA			B 416	-2.070 -21.031 12.000
40			- -	B 416	-2 819 -21.707 10.200
	MOTA	2816 C		B 416	-7 198 -23.1// 10.00 - ·
	MOTA	2817 CI		B 416	-() 9/3 -43·40/ -
	MOTA	2818 C		B 416	-0.405 -24.668 18.369 1.00 44.10 -0.305 25 541 17.346 1.00 41.85
	MOTA	2819 C		B 416	0 306 -20.041 -7.000
4:		2820 C		B 416	7 286 -24.700 -0.50-
	MOTA			B 416	-4 321 -21.645 18.559 1.00 36.55
	MOTA			B 416	-5 121 -21.790 17.638 1.00 38.30
	MOTA			B 417	-4.698 -41.430 43.00
	MOTA			B 417	-4.698 -21.435 20.196 1.00 36.46 -6.106 -21.371 20.196 1.00 36.46
5	MOTA 0			B 417	-6.218 -21.226 21.717 1.00 33.01
	ATOM		B CYS		-5.674 -22.710 22.612 1.00 43.01
	ATOM		G CYS		-6.899 -20.277 19.491 1.00 35.19
	MOTA			·	-8.127 -20.296 19.485 1.00 33.32
	MOTA				-6 195 -19.316 18.906 1.00 30.04
5	55 ATON	•	VAL		-6 838 -18.236 18.163 1.00 34.59
	ATO	•	CA VAL		-6.525 -16.850 18.775 1.00 34.87
	ATO	•	CB VAL	B 418	-6.831 -15.763 17.765 1.00 33.32
	ATO	M 2833	CG1 VAL	B 418	-7.350 -16.630 20.036 1.00 33.03
	ATO	M 2834	CG2 VAL	B 418	-6.241 -18.317 16.764 1.00 34.17
	60 ATO	м 2835	C VAL	B 418	-5.020 -18.323 16.611 1.00 32.73
	ATO		O VAL	B 418	J. 404

5	MOTA	2837	N	GLU	В	419	-7.084 -18.388 15.740 1.00 33.44
	ATOM	2838		GLU	В	419	-6.554 -18.500 14.390 1.00 34.52
	ATOM	2839	CB	GLU	В	419	-7.681 -18.722 13.380 1.00 36.21
	ATOM	2840	CG	GLU	В	419	-8.597 -17.538 13.166 1.00 44.19
	ATOM	2841	CD	GLU	В	419	-9.477 -17.723 11.946 1.00 48.47
10	ATOM	2842	OE1	GLU	В	419	-9.157 -18.605 11.119 1.00 51.04
	MOTA	2843	OE2	GLU	В	419	-10.484 -16.993 11.813 1.00 48.91
	ATOM	2844	С	GLU	В	419	-5.717 -17.289 13.997 1.00 32.89
	ATOM	2845	0	GLU	В	419	-6.156 -16.144 14.123 1.00 31.09
	ATOM	2846	N	GLY	В	420	-4.501 -17.562 13.535 1.00 32.84
15	ATOM	2847	CA	GLY	В	420	-3.594 -16.506 13.122 1.00 34.37
	ATOM	2848	С	GLY	В	420	-2.722 -15.955 14.240 1.00 35.30
	MOTA	2849	0	GLY	В	420	-1.745 -15.246 13.975 1.00 35.94
	ATOM	2850	N	MET	В	421	-3.052 -16.285 15.486 1.00 30.08
	ATOM	2851	CA	MET	В	421	-2.289 -15.780 16.625 1.00 29.22
20	ATOM	2852	CB	MET	В	421	-3.108 -15.922 17.914 1.00 22.54
	ATOM	2853	CG	MET	В	421	-2.469 -15.270 19.124 1.00 23.82
	ATOM	2854	SD	MET	В	421	-2.124 -13.494 18.872 1.00 28.40
	ATOM	2855	CE	MET	В	421	-3.697 -12.800 19.233 1.00 24.67
	MOTA	2856	С	MEŢ	В	421	-0.912 -16.416 16.821 1.00 29.67
25	MOTA	2857	0	MEŢ	₿	421	0.022 -15.751 17.269 1.00 29.76
	ATOM	2858	N	VAĻ	B	422	-0.766 -17.694 16.484 1.00 30.63
	MOTA	2859	CA	VAL	В	422	0.524 -18.338 16.675 1.00 29.90
	ATOM	2860		VAL	В	422	0.482 -19.835 16.273 1.00 35.74
••	ATOM	2861		٧ĄĮ	B	422	0.514 -19.992 14.753 1.00 37.64
30	MOTA	2862		٧ĄĻ	В	422	1.659 -20.555 16.897 1.00 31.68
	MOTA	2863		VAL	В	422	1.669 -17.640 15.935 1.00 28.64
	ATOM	2864		VAL	В	422	2.788 -17.571 16.441 1.00 26.15
	MOTA	2865	N	GLU	В	423	1.402 -17.113 14.747 1.00 28.70
25	ATOM	2866	CA	GĻÜ	₿	423	2.454 -16.435 13.997 1.00 31.34
35	MOTA	2867		GĽÜ	В	423	100 30.21
	ATOM	2868	CG	GLU	В	423	0.502 -16.376 12.325 1.00 45.83
	ATOM	2869	CD	GLU	В	423	0.250 -17.865 12.144 1.00 46.71
	ATOM	2870	OE1	GLU	В	423	-0.746 -18.368 12.706 1.00 45.97
40	ATOM	2871	OE2	GĻÜ	B	423	1.045 -18.530 11.442 1.00 50.05
40	ATOM ATOM	2872	C	GĽÜ	В	423	2.928 -15.186 14.744 1.00 30.57
		2873	0	GLU	В	423	4.119 -14.870 14.759 1.00 26.59
	ATOM ATOM	2874	N	ILE	В	424	2.001 -14.478 15.378 1.00 26.19
		2875		ILE	В	424	2.381 -13.279 16.111 1.00 26.23
45	ATOM ATOM	2876	CB	ILE	В	424	1.134 -12.435 16.452 1.00 29.33
73	ATOM	2877 2878	CG2	ILE	B	424	1.492 -11.315 17.425 1.00 30.91
	ATOM	2879	CG1	ILE	В	424	0.584 -11.817 15.160 1.00 29.09
	ATOM		CD1	ILE	В	424	-0.895 -11.514 15.187 1.00 30.51
	ATOM	2880 2881	C	ILE	В	424	3.153 -13.673 17.370 1.00 24.22
50	ATOM	2882	0	ILE	B	424	4.152 -13.037 17.725 1.00 21.05
50	ATOM	2883	N	PHÉ	В	425	2.708 -14.746 18.023 1.00 21.71
	ATOM	2884	CA	PHE	В	425	3.370 -15.236 19.223 1.00 18.85
	ATOM	2885	CB	PHE	В	425	2.650 -16.479 19.768 1.00 22.98
	ATOM	2886	CG	PHE	В	425	1.580 -16.183 20.795 1.00 22.17
55	ATOM	2887	CD1	PHE	В	425	1.287 -17.112 21.792 1.00 25.47
	ATOM		CD2	PHE	В	425	0.843 -15.001 20.747 1.00 26.30
	ATOM	2888 2889	CE1	PHE	В	425	0.273 -16.871 22.724 1.00 24.33
	ATOM	2890	CE2 CZ	PHE	В	425	-0.174 -14.749 21.676 1.00 25.03
	ATOM	2890	CZ	PHE	В	425	-0.459 -15.684 22.663 1.00 26.44
60	ATOM	2892	0	PHE	В	425	4.817 -15.610 18.885 1.00 20.00
	ATOM		N	PHE	В	425	5.741 -15.292 19.636 1.00 21.15
		2073	TA	ASP	В	426	5.023 -16.281 17.754 1.00 19.87

				_	6.378 -16.685 17.377 1.00 23.20
5	MOTA	2894 CA	ASP B	426	6 364 -17 510 16.090 1.00 26.53
	MOTA	2895 CB	ASP B	426	5.992 -18.965 16.335 1.00 34.28
	ATOM	2896 CG	ASP B	426	5 242 -19 467 17.455 1.00 35.24
	MOTA	2897 OD1	ASP B	426	1 400 1 00 31 49
	ATOM	2898 OD2	ASP B	426	5.448 -19.000 20.000 1 00 21.84
10		2899 C	ASP B	426	7.302 -13.403 1 00 21 55
10	MOTA	2900 0	ASP B	426	8.465 -13.326 -1 20 20 12
	ATOM	2901 N	MET B	427	6.788 -14.429 10.332 3 00 21.02
	MOTA	2902 CA	MET B	427	7.597 -13.234 100 100 10 53
	MOTA	2903 CB	MET B	427	6.836 -12.220 20 27 92
	ATOM	2904 CG	MET B	427	6.864 -12.339 14.000 - 1 00 32 84
15	MOTA		MET B	427	6.011 -11.341 13.021 - 1.00 33.63
	ATOM	2500	MET B	427	4 163 -11.332 +3.33-
	MOTA		MET B	427	7 945 -12.010 17.732
	MOTA		MET B	427	9 0/3 -12.100 17.50
	MOTA	2908 0	LEU B	428	6.968 -12.397 10.000
20	MOTA	2909 N	LEU B	428	7 15/ -12.033 13.300 -
	MOTA	2910 CA	LEU B	428	5.812 -11.964 20.706 1.00 17.58
	MOTA	2911 CB	LEU B	428	4.852 -10.887 20.179 1.00 18.41
	ATOM	2912 CG		428	3.443 -11.155 20.687 1.00 11.95
	MOTA	2913 CD1		428	5.324 -9.505 20.631 1.00 17.80
25	MOTA	2914 CD2	—	428	8 159 -12.856 20.767 1.00 20.88
	MOTA	2915 C		428	9.028 -12.305 21.445 1.00 20.45
	MOTA	2916 0		429	8.037 -14.178 20.679 1.00 20.33
	MOTA	2917 N			8.938 -15.082 21.382 1.00 19.82
	MOTA	2918 CA	• •		8 470 -16.532 21.211 1.00 23.13
30	MOTA	2919 CB	LEU B		7 189 -16.839 21.997 1.00 21.83
	MOTA	2920 CG	LEU B		6.551 -18.123 21.494 1.00 25.39
	MOTA	2921 CD			7 537 -16.944 23.475 1.00 24.91
	ATOM	2922 CD			10.361 -14.936 20.865 1.00 20.74
	MOTA	2923 C	LEU E		11 318 -14.968 21.638 1.00 21.02
35	MOTA	2924 0	rëñ e		10 495 -14.770 19.554 1.00 21.40
	MOTA	2925 N	ALA	_	11 808 -14.609 18.947 1.00 22.77
	MOTA	2926 CA		3 430	12 677 -14 596 17.432 1.00 21.11
	ATOM	2927 CB	-	B 430	13 315 19 440 1.00 22.40
	MOTA	2928 C		B 430	12 670 13 277 19 713 1.00 20.62
40		2929 O	1 44 11 7	B 430	12 258 19 567 1.00 21.09
,,	ATOM	2930 N	• • •	B 431	12 183 -10.974 20.021 1.00 22.67
	ATOM	2931 CF		B 431	11 128 -9.866 19.863 1.00 23.77
	MOTA	2932 CE	,	B 431	936 18 547 1.00 23.84
	MOTA	2933 00	_	B 431	11 762 -8 489 20.073 1.00 21.78
45		2934 C		B 431	12 603 -11 037 21.480 1.00 21.98
	ATOM	2935 C	- - . •	B 431	13 505 10 429 21 879 1.00 19.85
	ATOM	2936 O	THR	B 431	773 22 280 1.00 24.24
	ATOM	2937 N		B 432	
	ATOM		a ser	B 432	12 661 24 423 1.00 28.00
5			B SER	B 432	11.055 12.002 25.776 1.00 30.31
,	ATOM		G SER	B 432	11 404 -12.000 25.
	ATOM		SER	В 432	13.491 -12.000 23 78
	ATOM		SER	B 432	14.305 -12.377 24.70
	ATOM			B 433	13.691 -13.626 22.550
_			A SER	B 433	14.914 -14.421 22.520 1 00 30 84
5			B SER	B 433	14.790 -15.575 21.555
	MOTA		G SER	B 433	14.761 -16.808 22.025 - 1 00 31 47
	MOTA	•		B 433	16.104 -13.550 22.540 - 1 00 28 43
	ATON	•	SER	B 433	17 204 -13.701 23.00
	OTA	,	N ARG	в 434	15 878 -12.641 21.007
•	60 ATO		CA ARG	B 434	16.926 -11.739 21.165 1.00 29.40
	OTA	y 2330 '			

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5	MOTA	2951	CB	ARG	В	434	16.437	-10.912 19.977	1.00	31.56
	ATOM	2952	CG	ARG	В	434	17.428	-9.868 19.493	1.00	36.76
	ATOM	2953	CD	ARG	В	434	18.694	-10.502 18.919	1.00	37.76
	ATOM	2954	NE	ARG	В	434	19.654	-9.479 18.516	1.00	39.50
	MOTA	2955	CZ	ARG	В	434	20.965	-9.673 18.418	1.00	44.17
10	ATOM	2956	NHl	ARG	В	434	21.492	-10.861 18.696	1.00	43.17
	MOTA	2957	NH2	ARG	В	434	21.750	-8.671 18.048	1.00	43.05
	ATOM	2958	С	ARG	В	434	17.328		1.00	29.15
	ATOM	2959	0	ARG	В	434	18.515	_	1.00	28.82
	ATOM	2960	N	PHE	В	435	16.337		1.00	24.88
15	ATOM	2961	CA	PHE	В	435	16.600	-9.422 24.186	1.00	25.74
	ATOM	2962	CB	PHE	В	435	15.278	-8.972 24.825	1.00	
	ATOM	2963	CG	PHE	В	435	14.656	-7.758 24.183		26.53
	ATOM	2964	CD1	PHE	В	435	15.118		1.00	30.94
	ATOM	2965	CD2	PHE	В	435	13.592	-7.271 22.966 -7.108 24.797	1.00	32.65
20	MOTA	2966	CE1	PHE	В	435			1.00	33.60
20	ATOM	2967	CE2	PHE	В	435	14.529 12.997	-6.155 22.372	1.00	36.84
	ATOM	2968	CZ					-5.989 24.208	1.00	34.96
	MOTA	2969	C	PHE PHE	B B	435	13.468	-5.516 22.995	1.00	31.64
	MOTA	2970	0			435	17.426		1.00	25.39
25	ATOM	2971	И	PHË ARG	B	435	18.414	-9.675 25.764	1.00	22.59
23	ATOM	2972	CA	ARG	B	436	16.999		1.00	24.58
	ATOM	2973	CB	ARG	В	436 436	17.675	-12.253 26.503	1.00	30.25
	ATOM	2974	CG	ARG	B B	436	16.898 17.232	-13.569 26.662	1.00	33.32
	ATOM	2975	CD	ARG	В	436		-14.358 27.915	1.00	38.17
30	ATOM	2976	NE	ARG	B	436	16.135 15.646	-15.367 28.260	1.00	37.27
50	ATOM	2977	CZ	ARG	В	436	14.433		1.00	43.92
	ATOM	2978	NH1	ARG	В	436	13.578		1.00	46.68
	ATOM	2979	NH2	ARG	B B	436	14.074	· · · · ·	1.00	45.59
	ATOM	2980	C ·	ARG	₽ B	436	19.110	-12.531 26.048	1.00	46.25
35	ATOM	2981	0	ARG	B	436	20.057		1.00	29.82
55	ATOM	2982	И	AMET	B	437	19.269	-12.337 26.823	1.00 0.50	28.76
	ATOM	2983	N	BMET	В	437	19.252	-12.921 24.789	0.50	30.27
	ATOM	2984	CA	AMET	B	437	20.591		0.50	31.41
	ATOM	2985	CA	BMET	В	437	20.547		0.50	31.98
40	ATOM	2986	CB	AMET	В	437	20.489	-13.646 22.788		33.77
	ATOM	2987	CB	BMET	В	437	20.348	-13.595 22.714	0.50	31.34
	ATOM	2988	CG	AMET	B	437	20.179	-15.127 22.592	0.50	35.88
	ATOM	2989	CG	BMET	В	437	21.605		0.50 0.50	33.62
	ATOM	2990	SD	AMET	В	437		-16.099 24.109		40.47
45	ATOM	2991	SD	BMET	•	437		-13.937 20.115	0.50 0.50	35.21
	ATOM	2992	CE		В	437		-16.194 24.259		46.79
	ATOM	2993	CE		В	437		-15.632 19.976	0.50	33.20
	ATOM	2994	C	AMET	В	437		-11.993 24.366	0.50	43.22
	ATOM	2995	C	BMET	B	437		-12.005 24.289	0.50	33.33
50	ATOM	2996	0	AMET	B	437		-12.123 24.594	0.50	34.45
50	ATOM	2997	0	BMET	В	437			0.50	33.54
	ATOM	2998	N	MEŢ	В	438	20.913	-12.162 24.438 -10.809 24.215	0.50	34.43
	ATOM	2999	CA	MET		438	20.913		1.00	32.07
	ATOM	3000	CB		B B	438		-9.560 24.298	1.00	32.48
55	ATOM	3001	CG	MET MET	B B	438	20.930	-8.437 23.578	1.00	29.74
J J	ATOM	3001	SD	MET	B B		21.161	-8.364 22.093	1.00	36.73
	ATOM	3002	CE	MET	В	438 438	20.425	-6.849 21.462 -5.657 21.943	1.00	38.21
	ATOM	3004	CE	MET	В	438			1.00	35.91
	ATOM	3004	0	MET	B B		21.877	-9.122 25.738	1.00	28.81
60	ATOM	3006	и	ASN	B B	438 439	22.686 21.120	-8.240 26.013	1.00	30.13
	ATOM	3007		ASN_				-9.721 26.646	1.00	27.14
		J 5 0 /	CA	W214"	Þ	439	21.199	-9.359 28.038	1.00	27.34

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						20	22.592	-9.524		_	4.85
5	ATOM	3008 CB		SN B		39 39	22.532	-9.480			8.58
	ATOM	3009 CG		SN B		39 39	21.584	-9.620	30.724		2.99
	ATOM	3010 OD		SN B			23.801	-9.260	30.666		1.14
	ATOM	3011 ND		SN B		39 30	20.745	-7.903			6.24
	ATOM	3012 C		SN B		39	21.396	-7.106			19.76
10	ATOM	3013 0		SN B		39	19.625	-7.564	27.573		24.90
•	MOTA	3014 N		EU B		40	19.023	-6.214	27.633	1.00 2	25.04
	MOTA	3015 CA		EU B		40	17.761	-6.157	26.818		22.36
	ATOM	3016 CE		EU B		40	17.781	-4.786			26.33
	MOTA	3017 CG	} L	EU B		40	17.087	-3.843		1.00	28.33
15	ATOM	3018 CI		EU B		40	15.704	_4 914	26.111	1.00	24.81
	MOTA	3019 CI		EU B		140			29.074	1.00	24.71
	ATOM	3020 C	I	EU B		140	18.782	-6 504	29.830		26.96
	ATOM	3021 0		LEU B		140	18.131	-4 609	29.452	1.00	25.54
	ATOM	3022 N		SLN E		441	19.268		30.807		25.82
20	ATOM	3023 C	A (GLN E		441	19.060		31.234		30.41
20	ATOM	3024 C	в	GLN E		441	20.250		31.228	1.00	30.50
	ATOM	3025 C	G (GLN E		441	21.572		32.279	1.00	32.75
	ATOM		D (GLN F		441	21.610		33.473	1.00	36.52
	ATOM		E1 (GLN I	_	441	21.539	-4.172	31.823	1.00	31.09
25	ATOM		IE2	GLN 1		441	21.703		30.883	1.00	26.93
25	ATOM	3029 C	3			441	17.789		29.866	1.00	25.40
	ATOM	3030 C)	GLN :	Ŗ	441	17.303		32.096	1.00	24.56
	ATOM	3031 N	1		В	442	17.266	-3.10.	7 32.293	1.00	22.82
	ATOM		CA		B	442	16.058	-2.32 0 97	31.885		24.19
30	ATOM		2	GĻY	В	442	16.217		9 31.341		20.21
50	ATOM		C	GLY .	B	442	15.290		3 32.141		22.92
	MOTA		N	GLU.	В	443	17.387		2 31.778	1.00	23.33
	ATOM	3036	CA	GĹU	В	443	17.635		0 32.378		24.26
	MOTA	3037	CB	GLU	В	443	18.960		5 33.895		32.31
35	ATOM	3038	CG	GĻU	B	443	19.005		0 34.402		37.68
50	ATOM	3039	CD	GLU	В	443	19.701		1 33.948		35.23
	ATOM	3040	OE1	GLU	В	443	19.343		4 35.252		42.47
	MOTA	3041	OE2	GĽŪ	В	443	20.607		8 30.262		23.08
	ATOM	3042	C	GLŲ	В	443	17.662		8 29.74		21.80
40	ATOM	3043	0	GLU	В	443	17.265		3 29.55		21.16
	ATOM	3044	N	GĽÚ	₿	444	18.128		2 28.09		22.60
	ATOM	3045	CA	GLU	В	444	18.182		4 27.54		20.89
	ATOM	3046	CB	GLŪ	В	444	19.046	_	7 27.70		
	MOTA	3047	CG	GLU	В	444	20.545 21.34		9 27.39	3 1.00	22.11
45		3048	CD	GLU	В	444	20.81		78 27.62	9 1.00	20.89
	ATOM	3049	OE1	GLU	В	444	22.48		46 26.91		
	MOTA	3050	OE2	GĽÚ	В	444	16.75		55 27.55	2 1.00	21.06
	MOTA	3051	С	GLŲ	В	444			22 26.59	7 1.00	23.73
	ATOM	3052	0	GLU	В	444	16.37		30 28.17		
50		3053	N	PHE	B	445	15.98		69 27.79		
,	ATOM	3054	CA	PHE	В	445	14.60		67 28.67		
	ATOM	3055	CB	PHE	В	445	13.98		55 28.70		
	MOTA	3056	CG	PHE	В	445	12.48		86 27.57		
	MOTA	3057	CD1	PHE	В	445	11.74		00 4/.3/		
5:		3058	CD2	PHE	В	445	11.80		94 29.87		
٥.	MOTA C			PHE	В	445	10.34	_	59 27.59		
	ATOM			PHE	В	445	10.40	_	62 29.90		
	ATOM			PHE	В	445	9.67		97 28.7	-	
				PHE	В	445	13.75		04 27.8		
_	MOTA O			PHE	В	445	13.00		17 26.9		
0	MOTA 06 MOTA		-	VAL	В	446	13.8	72 1.0	44 28.9	00 1.0	
	AIOM	, 5.3.	- '								

5	ATOM	3065	CA	777 †	_	446	77 074	2 262 22 442		
,	ATOM	3065	CB	VAL	В	446	13.074	2.269 29.112	1.00	16.78
	ATOM	3067	CG1	VAL	B	446	13.165	2.895 30.531	1.00	18.32
	ATOM			VAL	В	446	12.574	1.923 31.551	1.00	21.14
		3068	CG2	VAL	В	446	14.598	3.251 30.879	1.00	21.04
10	MOTA MOTA	3069	C	VAL	В	446	13.450	3.295 28.051	1.00	17.91
10		3070	0	VAL	В	446	12.596	4.028 27.561	1.00	19.37
	ATOM	3071	N	CYS	В	447	14.723	3.335 27.674	1.00	18.81
	MOTA	3072	CA	CYS	В	447	15.161	4.255 26.635	1.00	17.34
	ATOM	3073	CB	CYS	В	447	16.682	4.224 26.512	1.00	19.33
15	MOTA	3074	SG	CYS	В	447	17.538	5.134 27.798	1.00	23.60
13	ATOM	3075	С	CYS	В	447	14.537	3.826 25.301	1.00	18.09
	MOTA	3076	0	CYS	В	447	13.988	4.643 24.563	1.00	17.52
	ATOM	3077	N	LEU	В	448	14.623	2.533 25.006	1.00	15.60
	ATOM	3078	CA	LEU	В	448	14.072	1.994 23.767	1.00	16.67
20	ATOM	3079	CB	LEU	В	448	14.328	0.490 23.684	1.00	14.82
20	MOTA	3080	CG	LEU	В	448	15.730	0.009 23.301	1.00	23.57
	ATOM	3081	CD1	LEU	B	448	15.722	-1.522 23.169	1.00	21.61
	ATOM	3082	CD2	LEU	В	448	16.167	0.658 21.986	1.00	18.92
	ATOM	3083	C	LEŲ	В	448	12.573	2.249 23.652	1.00	15.98
25	ATOM	3084	0	LEU	В	448	12.078	2.633 22.590	1.00	18.91
23	ATOM	3085	N	LYS	В	449	11.849	2.037 24.745	1.00	17.94
	ATOM	3086	CA	LYS	В	449	10.405	2.232 24.733	1.00	16.66
	ATOM	3087	CB	LYS	В	449	9.796	1.745 26.047	1.00	16.45
	ATOM	3088	CG	LYS	В	449	8.285	1.861 26.115	1.00	16.12
30	ATOM	3089	CD	LYS	В	449	7.730	0.952 27.193	1.00	19.09
30	ATOM	3090	CE	LYS	В	449	8.201	1.380 28.580	1.00	17.04
	MOTA MOTA	3091	NZ	LYS	В	449	7.159	1.088 29.593	1.00	17.25
	MOTA	3092 3093	С О	LYS	В	449	10.058	3.696 24.486	1.00	18.78
	ATOM	3094	N	LYS	В	449	9.103	3.996 23.769	1.00	14.84
35	ATOM	3094		SER	В	450	10.837	4.610 25.059	1.00	14.50
33	ATOM	3095	CA CB	SER SER	B B	450	10.591	6.032 24.849	1.00	17.11
	MOTA	3090	OG	SER		450	11.440	6.866 25.815	1.00	21.20
	ATOM	3098	C	SER	B B	450 450	10.859	6.868 27.108	1.00	30.66
	ATOM	3099	0	SER	В	450	10.921	6.418 23.405	1.00	17.84
40	ATOM	3100	N	ILE	В	451	10.279	7.292 22.821	1.00	18.82
-10	ATOM	3101	CA	ILE	В	451	11.926 12.305	5.768 22.828	1.00	16.88
	ATOM	3102	CB	ILE	В	451	13.564	6.063 21.450	1.00	17.11
	ATOM	3102	CG2	ILE	В	451	13.564	5.268 21.025	1.00	16.69
	ATOM	3104	CG1	ILE	В	451	14.804	5.298 19.505	1.00	19.31
45	ATOM	3105	CD1	ILE	В	451	16.083	5.897 21.676 5.130 21.431	1.00	18.96
	ATOM	3106	C	ILE	В	451	11.142	5.711 20.527	1.00	18.98
	ATOM	3107	0	ILE	В	451	10.820		1.00	18.09
	ATOM	3108	N	ILE	В	452		6.464 19.608	1.00	17.07
	ATOM	3109	CA	ILE	В	452	10.505 9.373	4.571 20.786	1.00	18.13
50	ATOM	3110	CB	ILE	В	452		4.137 19.976	1.00	16.77
50	ATOM	3111	CG2	ILE	В	452	8.804	2.775 20.477	1.00	17.40
	ATOM	3112	CG1	ILE	В	452	7.464	2.496 19.831	1.00	14.33
	ATOM	3113	CD1	ILE	В	452	9.763	1.635 20.107	1.00	15.36
	ATOM	3114	CDI	ILE	В	452	9.449	0.323 20.805	1.00	17.76
55	ATOM	3114	0	ILE	В	452 452	8.271	5.195 20.024	1.00	17.47
	ATOM	3115	N	LEU	В	452 453	7.733	5.586 18.992	1.00	16.50
	ATOM	3117	CA	LEU	В	453 453	7.943	5.665 21.222	1.00	16.06
	ATOM	3117	CB	LEU	В		6.903	6.680 21.374	1.00	17.17
	ATOM	3119	CG	LEU	В	453 453	6.736	7.061 22.850	1.00	16.23
60	ATOM	3119	CD1	LEU	В	453 453	5.792	8.228 23.163	1.00	17.60
	ATOM	3121	CD1	LEU	В	453 453	4.388	7.881 22.704	1.00	16.94
	ATOM	3441	CDZ	TEU	Þ	4 3 3	5.816	8.538 24.667	1.00	17.17

							7 100	7.941 20.566 1.00 19.3	3
5	ATOM	3122 C	L	EU B		53	7.198 6.320	9 458 19 879 1.00 21.3	
5	ATOM	3123 0	L	EU B		53		8.428 20.636 1.00 17.6	8
	MOTA	3124 N	I	J EU B		54	8.434	9.653 19.933 1.00 20.9	3
	MOTA		A I	JEU B		54	8.789	10.347 20.653 1.00 24.3	3
	ATOM	_		LEU B		154	9.959	10.699 22.130 1.00 26.1	
10	ATOM	-		LEU B	. 4	154	9.735	11.170 22.749 1.00 24.8	
10	MOTA			LEU B	. 4	154	11.046	11.777 22.259 1.00 23.7	
	ATOM			LEU B	3 4	454	8.658	9.494 18.449 1.00 20.7	
		3130		LEU E	3 4	454	9.120	J. 434 40. 440 - 1	
	ATOM		_	LEU E	3 4	454	8.941	10.431 17.00	
1.5	ATOM		-	ASN E	3 .	455	9.566	8.511 10.01	
15	MOTA			ASN I		455	9.951	0.000 20.000	
	MOTA					455	11.147	7.115 10.00	
	MOTA					455	11.576	0.071 23.23	
	ATOM		-		_	455	12.106	7.745 22.00	
	ATOM		ND2		_	455	11.343	3.010 =	
20	MOTA				В	455	8.925	7.580 15.655 1.00 22.	
	MOTA		C		В	455	8.790	8.127 14.564 1.00 21.	
	MOTA		0		В	456	8.224	6.514 16.023 1.00 25.	
	MOTA	3	N		B	456	7.260	5.873 15.135 1.00 24.	
	MOTA	3141	CA		В	456	6.402	4.894 15.939 1.00 26.	
25	MOTA	3142	CB	_	В	456	7.212	3.818 16.390 1.00 26.	
	MOTA	3143	OG	SER	В	456	6.385	6.774 14.272 1.00 26.	
	MOTA	3144	C	SER	В	456	6.323	6.588 13.055 1.00 29.	
	MOTA	3145	0	SER		457	5.716	7.750 ==	.07
	MOTA	3146	N	GLY	В	457	4.879	0.027 11.01	.19
30	MOTA	3147	CA	GLY	В	457	5.510	J. J. J. L.	.59
	MOTA	3148	С	GLY	В	457	4.851		.31
	MOTA	3149	0	GLY	В	458	6.789	10.130 14.092 1.00 31	.65
	MOTA	3150	N	VAL	В	458	7.486	TT.330 T3.0	.50
	ATOM	3151	CA	VAL	В	458	8.950	11 310 14.373 1.00 36	.24
35	MOTA	3152	CB	VAL	В	458	9.827	10 650 13.324 1.00 38	.50
	MOTA	3153	CG1	LAV	В		9.463	12.699 14.701 1.00 39	.84
	MOTA	3154	CG2	VAL	В	458	7.483	11 982 12.464 1.00 46	.30
	MOTA	3155	С	VAL	В	458	7.567	13,201 12,302 1.00 47	.67
	MOTA	3156	0	VAL	В	458	7.393	11.138 11.442 1.00 50	.45
40	MOTA	3157	N	TYR	В	459	7.385	11.640 10.069 1.00 57	7.07
	MOTA	3158		TYR	В	459	8.233	10.740 9.170 1.00 57	7.05
	ATOM	3159		TYR	В	459	9.673		29
	MOTA	3160	CG	TYR	В	459	10.284	11.786 10.203 1.00 60	93
	MOTA	3161	CD1	TYR	В	459	11.591	11.725 10.662 1.00 61	1.86
45	MOTA	3162	CE1	TYR	В	459	10.414	E	9.46
	MOTA	3163	CD2	TYR	В	459	11.726	9,439 9,943 1.00 59	9.67
	MOTA	3164	CE2	TYR	В	459	12.305		0.84
	ATOM	3165	CZ	TYR	В	459	13.593		1.39
	ATOM	3166	OH	TYR	В	459			1.22
50		316	7 C	TYR	В	459	5.97		2.89
•	MOTA	3168	3 0	TYR	В	459	5.62	7 12.,00	5.15
	ATOM	316		THR	В	460	5.16	6 10.730 3.700 -	7.76
	ATOM	317		THR	В	460	3.78	3 10.702 3.303 = 00 6	8.02
	ATOM	317		THR	В	460	3.17	8 9.203 3.202 =	7.03
<	5 ATOM	317			В	460	1.89	0 9.233 0.000 -	7.31
3	ATOM ATOM				В	460	3.04	0 0.510 10.550 -	0.14
				THR	В	460	2.94	5 11.700 10.207 1.00 7	2.35
	MOTA			THR		460	1.71	.5 11.041 40.000 - 00 7	72.64
	ATOM			PHE			3.62	5 12.020 10.700 -	75.05
	MOTA			PHE	_		2.96	13.03, 11.00	75.47
6	O ATOM			PHE			3.97	77 14.720 12.012 1.00 7	, , , , ,
	ATOM	, 31/	5 CB						

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5	ATOM	3179	CG	PHE	В	461	4.235	14.789 13.492	1.00	74.32
	MOTA	3180	CD1	PHE	В	461	3.200	14.609 14.404	1.00	73.98
	ATOM	3181	CD2	PHE	В	461	5.517	15.025 13.975	1.00	75.22
	MOTA	3182	CE1	PHE	В	461	3.438	14.662 15.775	1.00	74.02
	ATOM	3183	CE2	PHE	В	461	5.765	15.080 15.344	1.00	74.50
10	ATOM	3184	CZ	PHE	В	461	4.722	14.897 16.245	1.00	74.10
	ATOM	3185	С	PHE	В	461	1.787	14.286 10.896	1.00	76.78
	MOTA	3186	0	PHE	В	461	1.775	14.279 9.645	1.00	77.08
	ATOM	3187	CB	GLU	В	470	7.873	23.789 14.718	1.00	80.19
	MOTA	3188	C	GLU	В	470	8.958	21.731 15.650	1.00	79.30
15	ATOM	3189	0	GLU	В	470	9.887	21.518 16.432	1.00	78.21
	MOTA	3190	N	GLU	В	470	9.096	22.235 13.227	1.00	80.22
	MOTA	3191	CA	GLU	В	470	9.060	22.830 14.595	1.00	80.03
	ATOM	3192	N	GLU	В	471	7.823	21.037 15.665	1.00	78.31
	ATOM	3193	CA	GLU	В	471	7.596	19.956 16.617	1.00	75.83
20	ATOM	3194	CB	GLU	В	471	6.118	19.543 16.604	1.00	76.70
	ATOM	3195	CG	GLU	В	471	5.742	18.544 15.516	1.00	78.42
	MOTA	3196	CD	GLU	В	471	5.062	19.198 14.327	1.00	79.69
	ATOM	3197	OEl	GLU	В	471	3.829	19.398 14.378	1.00	80.26
	MOTA	3198	OE2	GLU	В	471	5.763	19.511 13.340	1.00	80.72
25	ATOM	3199	С	GLU	В	471	8.487	18.756 16.292	1.00	73.13
	ATOM	3200	0	GLU	В	471	8.897	18.021 17.189	1.00	73.86
	ATOM	3201	N	LYS	В	472	8.785	18.565 15.009	1.00	69.65
	ATOM	3202	CA	LYS	В	472	9.639	17.461 14.581	1.00	64.40
	MOTA	3203	CB	LYS	В	472	9.578	17.293 13.060	1.00	63.78
30	MOTA	3204	CG	LYS	В	472	8.343	16.552 12.566	1.00	64.49
	MOTA	3205	CD	LYS	В	472	8.544	16.002 11.161	1.00	63.81 64.90
	MOTA	3206	CE	LYS	В	472	7.379	16.368 10.249 15.212 9.990	1.00	63.97
	ATOM	3207		LYS	В	472	6.475	15.212 9.990 17.749 15.014	1.00	61.03
	ATOM	3208		LYS	В	472	11.071	16.833 15.287	1.00	60.28
35	ATOM	3209		LYS	В	472	11.848 11.413	19.033 15.076	1.00	56.84
	MOTA	3210		ASP	B B	473 473	12.745	19.451 15.488	1.00	51.69
	MOTA	3211		ASP ASP	В	473	12.743	20.940 15.242	1.00	50.36
	ATOM	3212		ASP ASP	В	473	12.923	19.138 16.970	1.00	49.18
40	MOTA	3213		ASP	В	473	13.959	18.619 17.385	1.00	46.85
40	MOTA	3214 3215		HIS	В	474	11.898	19.449 17.758	1.00	45.35
	MOTA	3215		HIS	В	474	11.923	19.203 19.196	1.00	43.65
	ATOM ATOM	3217		HIS	В	474	10.652	19.761 19.847	1.00	43.70
•	ATOM	3217		HIS	В	474	10.458	19.326 21.267	1.00	43.86
45	ATOM	3219		HIS	В	474	11.095	19.688 22.406		44.12
73	ATOM	3220		HIS	В	474	9.510	18.395 21.638		46.60
	ATOM	3221		HIS	В	474	9.572	18.202 22.943		45.29
	ATOM	3222		HIS	В	474	10.526	18.975 23.434		47.96
	ATOM	3223		HIS	В	474	12.030	17.707 19.471		42.38
50	ATOM	3224		HIS	В	474	12.834	17.273 20.298		42.83
30	ATOM	3225		ILE	В	475	11.214	16.923 18.773		38.86
	ATOM	3226		ILE	В	475	11.222	15.475 18.943		36.53
	ATOM	3227		ILE	В	475	10.105	14.822 18.110	1.00	36.56
	MOTA	3228		ILE	В	475	10.390	13.335 17.911		
55	ATOM	3229		ILE	В	475	8.770	14.998 18.832		35.81
22	ATOM	3230		ILE	В	475	7.598	14.410 18.094		41.77
	ATOM	3231		ILE	В	475	12.575	14.898 18.532		33.72
	ATOM	3232		ILE	В	475	13.112	14.023 19.207		31.50
	ATOM	3233		HIS	В	476	13.121	15.375 17.429		
60	ATOM	3234		HIS	В	476	14.421	14.886 16.992		33.31
30	ATOM	3235		HIS	В	476	14.782			37.30
					_					

5	ATOM	3236	CG	HIS	В	476	14.132	14.781 14.486	1.00	43.64
	MOTA	3237	CD2	HIS	В	476	13.723	13.498 14.342	1.00	45.25
	ATOM	3238	ND1	HIS	В	476	13.816	15.419 13.306	1.00	48.37
	ATOM	3239	CE1	HIS	В	476	13.238	14.560 12.484	1.00	48.87
	ATOM	3240	NE2	HIS	В	476	13.170	13.387 13.089	1.00	48.11
10	ATOM	3241	С	HIS	В	476	15.506	15.213 18.022	1.00	31.20
	ATOM	3242	0	HIS	В	476	16.442	14.436 18.208	1.00	27.25
	ATOM	3243	N	ARG	В	477	15.387	16.365 18.684	1.00	30.64
	ATOM	3244	CA	ARG	В	477	16.361	16.754 19.703	1.00	30.09
	ATOM	3245	CB	ARG	В	477	16.144	18.214 20.121	1.00	33.46
15	ATOM	3246	CG	ARG	В	477	16.322	19.212 18.982	1.00	40.74
10	ATOM	3247	CD	ARG	В	477	16.274	20.649 19.479	1.00	45.91
	ATOM	3248	NE	ARG	В	477	17.514	21.020 20.155	1.00	51.37
	ATOM	3249	CZ	ARG	В	477	18.375	21.927 19.702	1.00	53.68
	ATOM	3250	NH1	ARG	В	477	18.140	22.567 18.560	1.00	53.04
20	ATOM	3251	NH2	ARG	В	477	19.480	22.185 20.389	1.00	51.79
20	ATOM	3252	C	ARG	В	477	16.232	15.835 20.925	1.00	26.97
	ATOM	3252	0	ARG	В	477	17.233	15.387 21.486	1.00	27.34
		3254	N	VAL	В	478	14.999	15.558 21.338	1.00	23.70
	ATOM	3254	CA	VAL	В	478	14.780	14.685 22.482	1.00	24.79
25	ATOM		CB	VAL	В	478	13.286	14.613 22.861	1.00	24.83
23	ATOM	3256		LAV LAV	В	478	13.288	13.646 24.022	1.00	26.23
	ATOM	3257	CG1		В	478	12.781	15.996 23.243	1.00	28.26
	ATOM	3258	CG2	VAL			15.284	13.294 22.112	1.00	26.10
	ATOM	3259	C	VAL	В	478	15.204	12.613 22.927	1.00	24.28
20	MOTA	3260	0	VAL	В	478 479	15.021	12.889 20.870	1.00	22.92
30	ATOM	3261	N	LEU	В		15.456	11.584 20.379	1.00	21.96
	ATOM	3262	CA	LEU	В	479 479	14.992	11.372 18.930	1.00	22.63
	ATOM	3263	CB	LEU	В		13.575	10.798 18.756	1.00	20.82
	ATOM	3264	CG	LEU	В	479		10.689 17.274	1.00	22.53
25	ATOM	3265	CD1	LEU	В	479	13.231	9.440 19.420	1.00	23.08
35	ATOM	3266	CD2	LEU	В	479	13.495	11.471 20.453	1.00	21.90
	ATOM	3267	C	LEU	В	479	16.975	10.416 20.778	1.00	23.11
	ATOM	3268	0	LEU	В	479	17.506 17.675	12.560 20.143	1.00	23.11
	MOTA	3269	N	ASP	В	480		12.566 20.198	1.00	24.29
40	ATOM	3270	CA	ASP	В	480	19.141 19.692	13.889 19.649	1.00	26.88
40	ATOM	3271	CB	ASP	В	480		13.889 19.849	1.00	33.32
	ATOM	3272	CG	ASP	В	480	19.773 19.857	12.836 17.499	1.00	35.44
	ATOM	3273	OD1	ASP	В	480		15.022 17.563		
	ATOM	3274		ASP	В	480	19.757	12.406 21.656	1.00	24.13
15	ATOM	3275		ASP	В	480	19.590	11.697 21.956	1.00	
45 .	ATOM	3276		ASP	В	480	20.551	13.077 22.560	1.00	25.18
	ATOM	3277		LYS	В	481	18.887			
	ATOM	3278	CA	LYS	В	481	19.213	13.010 23.980	1.00	26.78
	MOTA	3279		LYS	В	481	18.262	13.898 24.785	1.00	31.37
50	ATOM	3280	CG	LYS	В	481	18.962	14.788 25.804	1.00	43.84
50	ATOM	3281	CD	LYS	В	481	18.780	14.260 27.219	1.00	46.08
	ATOM	3282	CE	LYS	В	481	20.120	13.928 27.865	1.00	50.99
	ATOM	3283		LYS	В	481	21.177	14.922 27.511	1.00	54.35
	MOTA	3284		LYS	В	481	19.124	11.575 24.495	1.00	26.87
	ATOM	3285		LYS	В	481	19.951	11.145 25.305	1.00	20.37
55	MOTA	3286		ILE	В	482	18.124	10.830 24.027	1.00	23.26
	MOTA	3287		ILE	В	482	17.981	9.452 24.472	1.00	21.07
	ATOM	3288	CB	ILE	В	482	16.655	8.828 24.015	1.00	19.80
	MOTA	3289		ILE	В	482	16.580	7.370 24.491	1.00	17.40
	MOTA	3290		ILE	В	482	15.479	9.606 24.602	1.00	17.16
60	ATOM	3291		ILE	В	482	14.136	9.209 23.991	1.00	19.43
	MOTA	3292	С	ILE	В	482	19.135	8.616 23.947	1.00	20.21

5	MOTA	3293	0	ILE	В	482	19.621	7.722 24.640	1.00	25.55
-	MOTA	3294	N	THR	В	483	19.569	8.896 22.722	1.00	21.89
	ATOM	3295	CA	THR	В	483	20.701	8.176 22.141	1.00	22.67
	ATOM	3296	CB	THR	В	483	21.030	8.662 20.695	1.00	23.34
	ATOM	3297	OG1	THR	В	483	19.890	8.475 19.851	1.00	27.33
10	ATOM	3298	CG2	THR	В	483	22.203	7.882 20.116	1.00	24.46
••	ATOM	3299	С	THR	В	483	21.913	8.441 23.035	1.00	23.51
	ATOM	3300	0	THR	В	483	22.650	7.520 23.381	1.00	27.01
	ATOM	3301	N	ASP	В	484	22.119	9.703 23.404	1.00	22.88
	ATOM	3302	CA	ASP	В	484	23.237	10.058 24.276	1.00	24.93
15	MOTA	3303	CB	ASP	В	484	23.201	11.546 24.652	1.00	28.69
13	ATOM	3304	CG	ASP	В	484	23.504	12.464 23.485	1.00	29.19
		3305	OD1	ASP	В	484	23.982	11.984 22.437	1.00	29.63
	ATOM	3305	OD2	ASP	В	484	23.256	13.681 23.627	1.00	32.02
	ATOM	3300	C C	ASP	В	484	23.125	9.249 25.567	1.00	24.40
20	ATOM		0	ASP	В	484	24.125	8.780 26.103	1.00	25.60
20	MOTA	3308			В	485	21.899	9.096 26.066	1.00	20.16
	ATOM	3309	N	THR	В	485	21.670	8.365 27.307	1.00	22.28
	ATOM	3310	CA	THR	В	485	20.203	8.521 27.763	1.00	24.64
	MOTA	3311	CB	THR			19.878	9.914 27.830	1.00	24.28
	MOTA	3312	OG1	THR	В	485	19.993	7.896 29.133	1.00	23.32
25	MOTA	3313	CG2	THR	В	485	22.017	6.881 27.188	1.00	22.13
	MOTA	3314	C	THR	В	485	22.574	6.284 28.115	1.00	23.30
	MOTA	3315	0	THR	В	485		6.290 26.045	1.00	23.08
	MOTA	3316		LEU	В	486	21.686	4.881 25.792	1.00	22.26
	MOTA	3317	CA	LEU	В	486	21.969	4.452 24.464	1.00	20.93
30	ATOM	3318	CB	LEU	В	486	21.346	4.031 24.533	1.00	24.92
	MOTA	3319		LEU	В	486	19.878	4.031 24.333	1.00	21.96
	MOTA	3320		LEU	В	486	19.295		1.00	23.90
	ATOM	3321		LEU	В	486	19.763	2.658 25.196 4.634 25.742	1.00	24.12
	MOTA	3322		LEU	В	486	23.477	3.681 26.334	1.00	24.02
35	MOTA	3323		LEU	В	486	23.984	5.490 25.022	1.00	24.53
	MOTA	3324	N	ILE	В	487	24.191			25.16
	MOTA	3325		ILE	В	487	25.640	5.345 24.913	1.00	25.57
	MOTA	3326	CB	ILE	B	487	26.207	6.379 23.899		24.54
	ATOM	3327	CG2	ILE	В	487	27.725	6.522 24.051	1.00	
40	ATOM	3328	CG1	ILE	В	487	25.857	5.936 22.470		25.63
	MOTA	3329	CD1	ILE	В	487	26.538	4.646 22.021	1.00	25.68
	ATOM	3330) C	ILE	В	487	26.275	5.518 26.307	1.00	23.60
	MOTA	3331	. 0	ILE	В	487	27.200	4.794 26.671	1.00	23.65
	ATOM	3332	N	HIS	В	488	25.755	6.456 27.081	1.00	
45	MOTA	3333	CA	HIS	В	488	26.251	6.720 28.431	1.00	
	MOTA	3334	L CB	HIS	В	488	25.450	7.871 29.041	1.00	
	MOTA	3335	G CG	HIS	В	488	25.818	8.196 30.455	1.00	
	ATOM	3336	CD2	HIS	В	488	25.245	7.838 31.629	1.00	
	ATOM	3337	7 ND1	HIS	В	488	26.869	9.025 30.779	1.00	
50	MOTA	3338		HIS	В	488	26.927	9.164 32.091	1.00	
	ATOM	3339		HIS	В	488	25.953	8.453 32.630	1.00	
	ATOM	3340		HIS	В	488	26.123	5.463 29.292	1.00	
	ATOM	334:		HIS	В	488	27.071	5.054 29.967	1.00	
	ATOM	3342		LEU	В	489	24.949	4.850 29.266	1.00	
55	ATOM	3343		LEU	В	489	24.715	3.642 30.040	1.00	
22	ATOM	3344		LEU	В	489	23.298	3.127 29.788	1.00	27.07
	ATOM	3349		LEU	В	489	22.158	3.909 30.445	1.00	31.71
	ATOM	334		LEU	В	489	20.827	3.516 29.799	1.00	28.08
		334		LEU	В	489	22.143	3.616 31.949	1.00	
۷0	MOTA			LEU	В	489	25.718	2.561 29.642	1.00	
60	ATOM	334	=	LEU	В	489	26.241	1.832 30.486	1.00	
	MOTA	334	, 0	TEO	D	407	20.2.			

5	ATOM	3350	N	MET	В	490	25.978	2.453 28.345		23.82
,	ATOM	3351	CA	MET	В	490	26.900	1.438 27.857		26.38
	ATOM	3352	CB	MET	В	490	26.775	1.306 26.336	1.00	27.29
	ATOM	3353	CG	MET	В	490	25.418	0.776 25.895	1.00	21.68
	ATOM	3354	SD	MET	В	490	25.208	0.739 24.106	1.00	26.30
10	ATOM	3355	CE	MET	В	490	23.461	0.412 24.022	1.00	19.66
10		3356	C	MET	В	490	28.341	1.743 28.247	1.00	26.42
	ATOM	3357	0	MET	В	490	29.109	0.833 28.574	1.00	24.76
	ATOM	3358	N	ALA	В	491	28.713	3.018 28.207	1.00	26.67
	MOTA	3359	CA	ALA	В	491	30.074	3.394 28.577	1.00	30.73
1.5	ATOM	3360	CB	ALA	В	491	30.299	4.882 28.335	1.00	26.66
15	ATOM	3361	CD	ALA	В	491	30.250	3.053 30.056	1.00	32.08
	ATOM		0	ALA	В	491	31.194	2.361 30.438	1.00	34.66
	MOTA	3362	N	LYS	В	492	29.316	3.523 30.878	1.00	33.17
	ATOM	3363	CA	LYS	В	492	29.354	3.267 32.309	1.00	32.82
20	MOTA	3364	CB	LYS	В	492	28.110	3.849 32.976	1.00	36.38
20	ATOM	3365		LYS	В	492	28.412	4.797 34.123	1.00	38.68
	ATOM	3366	CG		В	492	27.242	4.887 35.084	1.00	41.41
	MOTA	3367	CD	LYS	В	492	26.299	6.013 34.698	1.00	47.57
	ATOM	3368	CE	LYS	В	492	26.395	7.184 35.618	1.00	50.76
	MOTA	3369	NZ	LYS LYS	В	492	29.453	1.771 32.619	1.00	34.08
25	MOTA	3370	C		В	492	30.090	1.382 33.593	1.00	34.31
	MOTA	3371	0	LYS	В	493	28.835	0.935 31.788	1.00	32.03
	ATOM	3372	N	ALA	В	493	28.867	-0.510 31.998	1.00	30.70
	MOTA	3373	CA	ALA ALA	В	493	27.719	-1.181 31.245	.1.00	28.80
•	ATOM	3374			В	493	30.201	-1.156 31.606	1.00	33.75
30	MOTA	3375	C	ALA ALA	В	493	30.402	-2.356 31.819	1.00	30.53
	ATOM	3376		GLY	В	494	31.102	-0.372 31.020	1.00	33.50
	MOTA	3377		GLY	В	494	32.405	-0.903 30.656	1.00	33.71
	ATOM	3378		GLY	В	494	32.639	-1.360 29.230	1.00	34.40
2.5	ATOM	3379		GLY	В	494	33.663	-1.989 28.950	1.00	33.13
35	MOTA	3380		LEU	В	495	31.712	-1.056 28.326	1.00	31.76
	ATOM	3381		LEU	В	495	31.859	-1.452 26.925	1.00	30.57
	MOTA	3382		LEU	В	495	30.494	-1.415 26.216	1.00	30.67
	ATOM	3383		LEU	В	495	29.610	-2.675 26.256	1.00	29.59
40	ATOM	3384		LEU	В	495	29.315	-3.058 27.700	1.00	26.60
40	ATOM	3385		LEU	В	495	28.307	-2.416 25.501		27.52
	MOTA	3386		LEU	В	495	32.829	-0.515 26.202		30.53
	ATOM	3387		LEU	В	495	32.855	0.688 26.468		28.14
	ATOM	3388 3389		THR	В	496	33.628	-1.064 25.291		28.03
15	MOTA	3390		THR	В	496	34.567	-0.243 24.529	1.00	29.06
45	ATOM	339		THR	В	496	35.511	-1.095 23.665	1.00	29.40
	ATOM	3392		THR	В	496	34.753	-1.758 22.641		30.29
	ATOM	3393		THR	В	496	36.228	-2.122 24.515		28.12
	ATOM			THR	В	496	33.770	0.652 23.590		30.12
50	ATOM	3394 339!		THR	В	496	32.580	0.433 23.380		29.74
50		339		LEU	В	497	34.430	1.654 23.018		30.44
	MOTA			LEU	В	497	33.762	2.567 22.104		28.54
	MOTA	339		LEU	В	497	34.768	3.564 21.529		31.14
	ATOM	339		LEU	В	497	35.209	4.719 22.434		33.58
<i></i>	ATOM	339		LEU		497	36.120	5.659 21.652		31.42
55		340				497	33.992	5.469 22.942		35.08
	ATOM	340		LEU			33.095	1.800 20.96		
	ATOM	340		LEU			31.967	2.105 20.574		
	MOTA	340		GLN			33.798	0.797 20.44		
	ATOM	340		GLN			33.289	-0.009 19.34		
60		340		GLN			34.411	-0.876 18.77		
	MOTA	340	6 CB	GIN	8	4,70	J			

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5	ATOM	3407	CG	GLN	В	498	33.967	-1.796 17.645	1.00	32.67
	ATOM	3408	CD	GLN	В	498	34.965	-2.912 17.374	1.00	38.39
	ATOM	3409	OE1	GLN	В	498	35.737	-3.298 18.254	1.00	36.78
	MOTA	3410	NE2	GLN	В	498	34.953	-3.437 16.153	1.00	33.18
	ATOM	3411	С	GLN	В	498	32.112	-0.888 19.774	1.00	25.70
10	ATOM	3412	0	GLN	В	498	31.167	-1.076 19.009	1.00	25.35
. •	ATOM	3413	N	GLN	В	499	32.173	-1.434 20.986	1.00	24.01
	ATOM	3414	CA	GLN	В	499	31.093	-2.281 21.487	1.00	25.34
	ATOM	3415	CB	GLN	В	499	31.501		1.00	28.38
	ATOM	3416	CG	GLN	В	499	32.537	-4.056 22.669	1.00	29.13
15	MOTA	3417	CD	GLN	В	499	32.913		1.00	30.80
13	MOTA	3418	OE1	GLN	В	499	33.306		1.00	33.62
	ATOM	3419	NE2	GLN	В	499	32.797	-6.004 24.074	1.00	30.64
		3420	C	GLN	В	499	29.842	-1.430 21.693	1.00	25.70
	ATOM	3421	0	GLN	В	499	28.715		1.00	26.22
20	ATOM	3422	N	GLN	В	500	30.062		1.00	23.09
20	ATOM	3422	CA	GLN	В	500	28.989		1.00	23.53
	ATOM			GLN	В	500	29.564		1.00	26.17
	MOTA	3424		GLN	В	500	29.958		1.00	27.71
	MOTA	3425			В	500	30.812	_	1.00	29.32
	MOTA	3426		GLN		500	30.559		1.00	28.48
25	MOTA	3427		GLN	В	500	31.831		1.00	25.07
	ATOM	3428		GLN	В		28.151		1.00	24.24
	MOTA	3429		GLŅ	В	500	26.923		1.00	24.40
	MOTA	3430		GLN	В	500	28.790		1.00	23.08
	MOTA	3431		HIS	В	501			1.00	26.92
30	MOTA	3432		HIS	В	501	28.004		1.00	32.00
	MOTA	3433		HIS	В	501	28.791		1.00	36.97
	MOTA	3434		HIS	В	501	29.988		1.00	40.32
	MOTA	3435		HIS	В	501	30.122		1.00	37.88
	MOTA	3436		HIS	В	501	31.224		1.00	38.81
35	MOTA	3437		HIS	В	501	32.066		1.00	41.21
	ATOM	3438		HIS	В	501	31.422		1.00	25.91
	MOTA	3439	C	HIS	В	501	27.45		1.00	20.13
	MOTA	3440	0	HIS	В	501	26.36	·	1.00	24.94
	MOTA	3441	LN	GLN	В	502	28.16		1.00	21.88
40	MOTA	3442	2 CA	GLN	В	502	27.69			
	ATOM	3443	3 CB	GLN	В	502	28.78		1.00	24.62 26.55
	MOTA	3444	4 CG	GLN	В	502	29.79			
	MOTA	3445	5 CD	GLN	В	502	30.84			27.06
	ATOM	3446	6 OE1	GLN	В	502	30.71			28.49
45	ATOM	344'	7 NE2	GLN	В	502	31.88			
	ATOM	344	8 C	GLN	В	502	26.42			
	MOTA	344	9 0	GĽŃ	B	502	25.46			
	MOTA	345	0 N	ARG	В	503	26.42			
	ATOM	345		ARG	В	503	25.25			
50	ATOM	345		ARG	В	503	25.60			
50	ATOM	345		ARG	В	503	24.45			
	ATOM	345		ARG	В	503	24.85			
	ATOM	345		ARG	В	503	23.74	3 -3.546 25.395		
	ATOM	345		ARG	В	503	23.32		1.00	
55	ATOM	345		ARG	В	503	23.93		1.00	16.40
دد		345		ARG	В	503	22.30			19.71
	ATOM			ARG	В	503	24.10			
	MOTA	345	=	ARG	В	503	22.94			
	ATOM	346				504	24.41			
	MOTA	346		LEU	В		23.37			
60	MOTA	346		LEU	В		23.97			
	MOTA	346	3 CB	LEU	В	504	23.31	,,	·-•	

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5	MOTA	3464	CG	LEU	В	504		.983		19.344	1.00	20.35
	MOTA	3465	CD1	LEU	В	504		.930		20.427	1.00	17.97
	ATOM	3466	CD2	LEU	В	504		.729		18.955	1.00	20.86
	ATOM	3467	C.	LEU	В	504		.659		18.667	1.00	21.22
	MOTA	3468	0	LEU	В	504		433		18.566	1.00	19.28
10	ATOM	3469	N	ALA	В	505	23	.428		17.676	1.00	18.55
	MOTA	3470	CA	ALA	В	505	22	2.859		16.396	1.00	18.20
	ATOM	3471	CB	ALA	В	505	23	3.973		15.382	1.00	18.45
	ATOM	3472	С	ALA	В	50 5		.986	-1.716	16.562	1.00	19.54
	ATOM	3473	0	ALA	В	505	20	.871		16.041	1.00	17.63
15	ATOM	3474	N	GLN	В	506	22	2.497	-2.706	17.293	1.00	20.30
	ATOM	3475	CA	GLN	В	506	2:	L.772		17.513	1.00	19.48
	ATOM	3476	CB	GLN	В	506	22	2.590		18.409	1.00	21.75
	ATOM	3477	CG	GLN	В	506	2:	3.798	-5.551	17.727	1.00	20.85
	ATOM	3478	CD	GLN	В	506	24	1.819	-6.070	18.736	1.00	26.18
20	ATOM	3479	OE1	GLN	В	506		1.564	-6.084	19.943	1.00	21.83
20	ATOM	3480	NE2	GLN	В	506		5.977	-6.499	18.245.	1.00	25.39
	ATOM	3481	C	GLN	В	506		0.421		18.166	1.00	21.39
	ATOM	3482	0	GLŅ	В	506		9.396		17.766	1.00	20.87
	ATOM	3483	N	LEU	В	507		0.433		19.171	1.00	19.52
25		3484	CA	LEU	В	507		9.219		19.884	1.00	23.04
23	MOTA	3485	CB	LEU	В	507		9.548		21.030	1.00	22.82
	MOTA		CG	LEU	В	507		0.182		22.313	1.00	26.12
	ATOM	3486		LEU	В	507		0.203		23.360	1.00	29.33
	ATOM	3487	CD1	LEU	В	507		9.415		22.816	1.00	27.80
20	ATOM	3488		LEU	В	507		8.212		18.971	1.00	22.19
30	ATOM	3489		LEU	В	507		7.036		18.964	1.00	23.00
	ATOM	3490		LEU	В	508		8.678		18.214	100	21.53
	ATOM	3491		LEU	В	508		7.797		17.332	1.00	20.60
	ATOM	3492		LEU	В	508		8.535		16.805	1.00	17.57
25	MOTA	3493		LEU	B	508		8.934		3 17.913	1.00	17.67
35	MOTA	3494		LEU	B	508		9.566		17.301	1.00	20.04
	MOTA	3495		LEU	В	508		7.724		18.725	1.00	18.49
	MOTA	3496		PEA	В	508		7.235		16.183	1.00	21.17
	MOTA	3497	-	LEÙ	В	508		6.118		7 15.728	1.00	21.88
40	ATOM	3498		LEÙ	B	509		8.000		15.713	1.00	21.89
40	ATOM	3499			B	509		7.511		7 14.631	1.00	22.81
	ATOM	3500		LEU	В	509		8.603		7 14.145	1.00	22.65
	ATOM	3501			В	509		9.645		13.278	1.00	29.11
	ATOM	3502		LEU		509		0.697		3 12.829	1.00	25.69
45	ATOM	3503		LEU	B B	509		8.965		3 12.082	1.00	27.92
45	ATOM	3504		LEU	В	509		6.302		2 15.095	1.00	23.32
	MOTA	3505		LEU	В	509		5.409		9 14.303	1.00	23.36
	ATOM	3506		LEU		510		6.264		5 16.380	1.00	23.36
	MOTA	3507		ILE	В			5.148		2 16.912	1.00	20.99
	ATOM	3508		ILE	В	510				1 18.361	1.00	28.60
50	MOTA	3509		ILE	В	510		.5.448		5 19.075	1.00	
	ATOM	3510		ILE	B	510		4.162			1.00	
	ATOM	3513		ILE	В	510		6.383		0 18.308	1.00	
	ATOM	3512		ILE	В	510		.7.429		1 19.419	1.00	
	ATOM	3513		ILE	В	510		3.852		6 16.846	1.00	
55	ATOM	3514		ILE	В	510		2.767		8 16.759		
	ATOM	3515		LEU	В	511		3.961		1 16.867	1.00	
	MOTA	3516		LEU	В	511		2.772		4 16.774		
	ATOM	351		LEU	В	511		13.147		0 16.981		
	ATOM	3518		LEU	В	511		13.607		2 18.406	1.00	
60	ATOM	3519	9 CD1	LEU	В	511		13.404		1 18.652	1.00	
	ATOM	3520	CD2	LEU	В	511		12.830	-0.54	9 19.425	1.00	25.08

5	MOTA	3521	С	LEU	В	511	12.11	_	-1.771 1	_		16.65
_	ATOM	3522	0	LEU	В	511	10.91		-1.578 1			17.09 15.83
	ATOM	3523	N	SER	В	512	12.90		-2.161 1			18.66
	ATOM	3524	CA	SER	В	512	12.35		-2.408			17.62
	ATOM	3525	CB	SER	В	512	13.48		-2.644		1.00	32.77
10	ATOM	3526	OG	SER	В	512	13.07		-3.550		1.00	
. •	ATOM	3527	С	SER	В	512	11.45		-3.638		1.00	18.54
	ATOM	3528	0	SER	В	512	10.37		-3.683		1.00	17.01
	ATOM	3529	N	HIS	В	513	11.89		-4.625		1.00	15.54
	MOTA	3530	CA	HIS	В	513	11.14		-5.860		1.00	17.67
15	ATOM	3531	CB	HIS	В	513	12.0		-6.916		1.00	19.03
	ATOM	3532	CG	HIS	В	513	13.06		-7.475		1.00	27.06
	ATOM	3533	CD2	HIS	В	513	12.98		-8.364		1.00	28.40
	ATOM	3534	ND1	HIS	В	513	14.37		-7.066		1.00	28.92
	ATOM	3535	CE1	HIS	В	513	15.06		-7.678		1.00	30.75
20	ATOM	3536	NE2	HIS	В	513	14.2		-8.472		1.00	30.08
	ATOM	3537	С	HIS	В	513	9.8		-5.602		1.00	15.35
	ATOM	3538	0	HIS	В	513	8.8		-6.192		1.00	14.83
	MOTA	3539		ILE	В	514	10.0		-4.744		1.00	13.35
	ATOM	3540	CA	ILE	В	514	8.8		-4.417		1.00	15.48
25	ATOM	3541	CB	ILE	В	514	9.2		-3.534		1.00	20.02
	MOTA	3542	CG2	ΙĻΕ	В	514	8.0		-2.918		1.00	12.84 22.87
	ATOM	3543	CG1	ILĖ	В	514	10.0		-4.397		1.00	29.62
	MOTA	3544	CD1	ILE	В	514	10.6		-3.641		1.00 1.00	15.16
	MOTA	3545	C	ILE	В	514	7.7		-3.717		1.00	16.61
30	MOTA	3546	0	ILE	В	514	6.6		-3.972	16.078	1.00	16.33
	ATOM	3547	N	ARĢ	В	515	8.2			15.030	1.00	17.54
	MOTA	3548	CA	ARG	В	515	7.2			14.150 13.214	1.00	20.15
	MOTA	3549	CB	ARG	В	515	8.0			12.234	1.00	21.47
	MOTA	3550		ARG	В	515	7.0			12.891	1.00	26.05
35	MOTA	3551		ARG	В	515	6.4			12.716	1.00	24.91
	MOTA	3552		ARG	В	515	7.2			12.547	1.00	24.61
	MOTA	3553		ARĢ	В	515	6.7			12.522	1.00	22.46
	MOTA	3554		ARG	В	515		124 569		12.374	1.00	23.15
	MOTA	355		ARG	В	515		545		13.304	1.00	16.60
40	MOTA	355		ARG	-B	515		332		13.087	1.00	14.51
	ATOM	355		ARG	В	515		298		12.827	1.00	18.50
	MOTA	355		HIS	В	516		743		11.997		
	MOTA	355		HIS	В	516		861		11.533	1.00	
	ATOM	356		HIS	В	516 516		405		10.568		
45	ATOM	356		HIS	В	516		060		10.754		26.64
	ATOM	356			В	516		258	-6.978			
	MOTA	356			В	516		839	-8.078			28.42
	MOTA	356			В	516		711	-9.028			
	MOTA	356			В	516		685		12.759		
50		356		HIS	В	516		596		12.240		
	ATOM	356		HIS	В	517		999		13.997		
	MOTA	356		MET	В	517		049		14.801		
	MOTA	356		MET	В	517		701		7 16.114		
	ATOM	357		MET	В			790		3 15.917		
55		357		MET				380		17.470		
	ATOM	357		MET				104		9 18.226		
	ATOM	357		MET				789		3 15.080		
	ATOM	357		MET				688		4 15.148		
	ATOM	357		MET				954		0 15.247		
60		357		SER				827		6 15.505		
	MOTA	357	77 CA	SER		210	ے.					

5	ATOM	3578	CB	SER	В	518	3.316	-2.765 15.835	1.00	17.48
	ATOM	3579	OG	SER	В	518	2.234	-1.840 15.843	1.00	17.46
	ATOM	3580	С	SER	В	518	1.906	-4.147 14.284	1.00	14.73
	ATOM	3581	0	SER	В	518	0.688	-4.247 14.417	1.00	19.16
	ATOM	3582	N	ASN	В	519	2.474	-4.006 13.091	1.00	14.52
10	ATOM	3583	CA	ASN	В	519	1.622	-3.953 11.907	1.00	15.35
	MOTA	3584	CB	ASN	В	519	2.432	-3.509 10.698	1.00	19.21
	ATOM	3585	CG	ASN	В	519	2.700	-2.029 10.729	1.00	20.58
	ATOM	3586	OD1	ASN	В	519	1.839	-1.258 11.150	1.00	26.36
			ND2	ASN	В	519	3.891	-1.618 10.307	1.00	19.62
15	ATOM	3587								
13	ATOM	3588	C	ASN	В	519	0.911	-5.280 11.658	1.00	16.74
	ATOM	3589	0	ASN	B	519	-0.265	-5.299 11.297	1.00	20.58
	ATOM	3590	N	LYS	В	520	1.608	-6.387 11.885	1.00	18.60
	ATOM	3591	CA	LYS	В	520	0.992	-7.699 11.717	1.00	20.04
	ATOM	3592	CB	LYS	В	520	2.038	-8.801 11.872	1.00	25.44
20	ATOM	3593	CG	LYS	В	520	3.037	-8.849 10.728	1.00	31.68
	ATOM	3594	CD	LYS	В	520	2.507	-9.663 9.558	1.00	42.56
	ATOM	3595	CE	LYS	В	520	2.186	-8.778 8.364	1.00	45.61
	ATOM	3596	NZ	LYS	B	520	1.435	-9.526 7.312	1.00	46.00
	ATOM	3597	C	LYS	В	520	-0.099	-7.868 12.769	1.00	18.88
25	ATOM	3598	0	LYS	В	520	-1.183	-8.358 12.478	1.00	21.75
	ATOM	3599	N	GLY	В	521	0.191	-7.455 13.998	1.00	17.83
	ATOM	3600	CA	GLY	В	521	-0.792	-7.569 15.058	1.00	16.19
	ATOM	3601	ď	GLY	В	521	-2.000	-6.674 14.833	1.00	16.59
	ATOM	3602	0	GLY	В	521	-3.128	-7.060 15.125	1.00	16.57
30	ATOM	3603	N	MET	В	522	-1.766	-5.467 14.326	1.00	17.48
	ATOM	3604	CA	MET	В	522	-2.852	-4.527 14.042	1.00	18.25
	ATOM	3605	CB	MET	В	522	-2.276	-3.212 13.516	1.00	21.27
	ATOM	3606	CG	MET	В	522	-3.190	-2.018 13.707	1.00	26.97
	MOTA	3607	SD	MET	В	522	-3.199	-1.477 15.417	1.00	30.35
35	ATOM	3608	CE	MET	В	522	-1.659	-0.605 15.475	1.00	29.86
	ATOM	3609	C	MET	В	522	-3.794	-5.119 12.989	1.00	18.68
	ATOM	3610	Ō	MET	В	522	-5.022	-5.008 13.097	1.00	18.80
	ATOM	3611	N	GLU	В	523	-3.205	-5.731 11.966	1.00	18.22
	ATOM	3612	CA	GLU	В	523	-3.968	-6.357 10.889	1.00	23.41
40	ATOM	3613	CB	GLU	В	523	-3.031	-6.946 9.830	1.00	28.74
	ATOM	3614	CG	GLU	В	523	-2.224	-5.935 9.030	1.00	34.42
	ATOM	3615	CD	GLU	В	523	-1.095	-6.597 8.239	1.00	45.58
	ATOM	3616	OE1	GLU	В	523	-0.131	-5.894 7.857	1.00	49.48
	ATOM	3617	OE2	GLU	В	523	-1.169	-7.825 7.999	1.00	45.97
45	ATOM	3618	C	GLU	В	523	-4.812	-7.482 11.465	1.00	23.98
7.5	ATOM	3619	0	GLU	В	523	-5.993	-7.616 11.147	1.00	22.08
	MOTA	3620	N	HIS	В	524	-4.187	-8.287 12.326	1.00	23.46
	ATOM	3621	CA	HIS	В	524	-4.846	-9.428 12.952		26.20
									1.00	
50	ATOM	3622	CB	HIS	В	524	-3.824	-10.245 13.743	1.00	27.26
30	ATOM	3623	CG	HIS	В	524	-4.378	-11.509 14.321	1.00	30.91
	ATOM	3624	CD2	HIS	B	524	-4.308	-12.792 13.892	1.00	30.90
	ATOM	3625	ND1	HIS	В	524	-5.107	-11.537 15.490	1.00	28.87
	MOTA	3626	CE1	HIS	В	524	-5.461	-12.780 15.757	1.00	30.45
<i></i>	MOTA	3627	NE2	HIS	В	524	-4.989	-13.561 14.803	1.00	29.19
55	ATOM	3628	С	HIS	В	524	-5.996	-9.025 13.870	1.00	27.69
	ATOM	3629	0	HIS	В	524	-7.061	-9.656 13.860	1.00	25.00
	ATOM	3630	N	LEU	В	525	-5.777	-7.977 14.655	1.00	23.84
	ATOM	3631	CA	LEU	В	525	-6.786	-7.492 15.588	1.00	25.77
	ATOM	3632	CB	LEU	В	525	-6.217	-6.358 16.444	1.00	22.22
60	ATOM	3633	CG	LEU	В	525	-7.164	-5.778 17.498	1.00	26.81
	ATOM	3634	CD1	LEU	В	525	-7.763	-6.922 18.321	1.00	23.32

5	ATOM	3635		LEU	В	525	-6.414	-4.79	3 18.399	9 1.00	18.95
	ATOM	3636		LEU	В	525	-8.013		5 14.842		
	ATOM	3637		LEU	В	525	-9.154		7 15.249		
	ATOM	3638		TYR	В	526	-7.764		1 13.757		
• •	ATOM	3639	CA	TYR	В	526	-8.819		6 12.918		
10	ATOM	3640	CB	TYR	В	526	-8.201		B 11.854		
	ATOM	3641	CG	TYR	В	526	-9.183		3 10.878		
	ATOM	3642	CD1	TYR	В	526	-10.058		1 11.267		
	MOTA	3643	CE1	TYR	В	526	-10.943		5 10.357		
	ATOM	3644	CD2	TYR	В	526	-9.218				
15	ATOM	3645	CE2	TYR	В	526	-10.098				
	ATOM	3646		TYR	В	526	-10.955	-3.07			
	ATOM	3647		TYR	В	526	-11.810			-	
	ATOM	3648		TYR	В	526	-9.577				
	ATOM	3649		TYR	В	526			12.265	-	
20	ATOM	3650	N	SER	В	527	-10.793		12.113		
	ATOM	3651	CA	SER			-8:849		11.889		
	ATOM	3652	CB	SER	В	527	-9.460		11.266		33.73
	ATOM	3653	OG	SER	В	527			10.749		34.13
	ATOM	3654	C		В	527			10.196		43.67
25	ATOM	3655	0	SER	В	527	-10.339		12.288	1.00	34.34
	ATOM	3656	Ŋ	SER	В	527	-11.446			1.00	33.42
	ATOM	3657		MET	В	528	-9.840		13.517	1.00	31.66
	ATOM	3658	CA	MET	В	528	-10.574			1.00	29.77
	ATOM		CB	MET	В	528			15.820	1.00	32.96
30	ATOM	3659	CG	MET	В	528			15.699	1.00	33.47
30	ATOM	3660	SD	MET	В	528	-9.359		15.134	1.00	38.28
		3661	CE	MET	В	528	-10.265	-13.915		1.00	36.01
	ATOM	3662	C	MET	В	528	-11.800		14.953	1.00	29.42
	ATOM	3663	0	MET	В	528	-12.835	-10.293	15.331	1.00	28.65
35	ATOM	3664	N	LYŚ	В	529	-11.673	-8.429	14.850	1.00	30.64
33	ATOM	3665	CA	LYS	В	529	-12.781	-7.533	15.149	1.00	31.80
	ATOM	3666	CB	LYS	В	529	-12.323	-6.079	15.027	1.00	32.86
	ATOM	3667	CG	LYS	В	529	-13.436	-5.043	15.114	1.00	36.42
	ATOM	3668	CD	LYS	В	529	-13.114		14.224	1.00	41.74
40	ATOM	3669	CE	LYS	В	529	-13.734		14.741	1.00	43.45
40	ATOM	3670	NZ	LYS	В	529	-15.221		14.634	1.00	46.51
	ATOM	3671	C	LYS	В	529	-13.857		14.116	1.00	36.60
	ATOM	3672	0	LYS	В	529	-15.049		14.424	1.00	34.04
	ATOM	3673	N	CYS	B	530	-13.407		12.889		40.04
4.5	ATOM	3674	CA	CYS	В	530	-14.286		11.773	1.00	44.58
45	ATOM	3675	CB	CYS	В	530	-13.460		10.491	1.00	50.64
	ATOM	3676	SG	CYS	В	530	-13.369	-7.034		1.00	
	ATOM	3677	C	CYS	В	530	-15.065		12.016	1.00	67.65
	ATOM	3678	0	CYS	В	530	-16.274		11.807		42.88
	ATOM	3679	N .	LYS	В	531		-10.733		1.00	40.15
50	ATOM	3680	CA	LYS	В	531	-14.980			1.00	41.92
	ATOM	3681	CB	LYS	В	531				1.00	42.60
	ATOM	3682	C	LYS	В	531	-13.907			1.00	44.77
	ATOM		0	LYS	В	531	-15.844			1.00	44.43
	ATOM		N	ASN	В		-16.623			1.00	44.09
55	ATOM		CA	ASN	В	532 532	-15.678	-10.793	14.685	1.00	44.98
*	ATOM	_	CB	ASN		532	-16.437			1.00	44.10
	ATOM		CG		В	532	-17.833			1.00	45.14
	ATOM			ASN	В	532		-9.271		1.00	46.54
	ATOM		OD1	ASN	В	532		-9.424		1.00	50.62
60	ATOM		ND2	ASŅ	В	532	-17.771	-8.471	17.375	1.00	46.07
50	ATOM		C	ASN	В	532	-16.557 -	-11.657	16.882	1.00	43.34
	ATOM	3691	U	ASN	В	532	-17.655 -	11.994	17.321	1.00	41.42

			_			533	-15.434 -		.45
5	MOTA	3692 N		VAL I	-	533		13.371 18.190 1.00 44	.06
	MOTA					533 533		14,219 18,120 1.00 45	5.56
	MOTA				_	533	-13.661 -	14.263 16.683 1.00 45	5.67
	ATOM			•••	-	533		13.644 19.045 1.00 44	1.16
	MOTA					533	-15.670 -	12.835 19.611 1.00 43	3.24
10	ATOM	• • •	_		В	533	-15.894 -	13.602 20.548 1.00 44	4.21
	MOTA		-		В		-15.596 -	11.511 19.755 1.00 40	0.44
	MOTA				В	534 . 534	-15.765 -	.10.849 21.049 1.00 3	7.80
	ATOM		CA		В		-14.630 -	11.259 22.038 1.00 3	6.38
	MOTA		CB		В	534	-13.324 -	-10.575 21.658 1.00 3·	4.35
15	MOTA		CG1	VAL	В	534	-15.021	-10.910 23.463 1.00 3	9.34
	MOTA		CG2	VAL	В	534	-15.752	-9.329 20.857 1.00 3	7.97
	ATOM		C	LAV	В	534	-15.026	-8.808 20.008 1.00 3	9.45
	MOTA	3705	0	VAL	В	534	-16.575	-8.597 21.625 1.00 3	7.81
	MOTA	3706	N	PRO	В	535	-17.529	-9.078 22.640 1.00 3	8.74
20	ATOM	3707	CD	PRO	В	535	-16.608	-7.135 21.492 1.00 3	6.79
	ATOM	3708	CA	PRO	В	535			6.98
	ATOM	3709	CB	PRO	В	535	-17.846 -18.004		39.77
	ATOM	3710	CG	PRO	В	535			33.95
	MOTA	3711	С	PRO	В	535	-15.338		34.93
25	ATOM	3712	0	PRO	В	535	-14.786		33.42
	ATOM	3713	N	LEU	В	536	-14.881		33.40
	ATOM	3714	CA	ΓĖŪ	В	536	-13.675		29.31
	ATOM	3715	CB	LEU	В	536	-12.829		30.06
	ATOM	3716	CG	LEU	В	536	-12.219		30.85
30	ATOM	3717	CD1	ĿĔŨ	В	536	-11.344		28.96
	ATOM	3718	CD2	ĻĒŪ	В	536	-11.398	-6.5/0 20.0/0	30.50
	ATOM	3719	С	LEU	В	536	-14.036	-3.400 22.00	29.91
	ATOM	3720	0	LEU	В	536	-15.024	-2.025 22.005 -	28.69
	ATOM	3721	N	TYR	В	537	-13.231	-3.194 23.070	29.89
35	ATOM	3722	CA	TŸŖ	В	537	-13.494	-2.052 21.505 -	32.50
20	ATOM	3723	CB	TYR	В	537	-12.618		39.46
	ATOM	3724	CG	TYR	В	537	-12.849	-3.431 27.421 1.00	41.90
	ATOM	3725	CD1	TYR	В	537	-13.923	-4.609 28.118 1.00	45.72
	ATOM	3726		TYR	В	537	-14.174	-4.435 26.379 1.00	47.39
40		3727		TYR	В	537	-12.022	-5.620 27.072 1.00	49.93
40	ATOM	3728		TYR	В	5 37	-12.262	-5.699 27.940 1.00	48.80
	ATOM	3729		TYR	В	537	-13.340	-6.872 28.624 1.00	53.90
	ATOM		OH	TYR	В	537	-13.582		27.09
	ATOM	3731		TYR	В	537	-13.262	1 00	26.15
45		3732		TYR	В	537	-12.518		26.12
72	ATOM	3733		ASP	В	538	-13.909	0.515 1101	25.27
	ATOM	3734		ASP	В	538	-13.830	1.000 1 00	28.85
	ATOM	3735		ASP	В	538	-14.748	2.555 2010 1 00	33.90
	ATOM	3736		ASP	В	538	-16.227	2.200 00 12	32.68
50		373		ASP	В	538	-17.052	2.015 2010 1 00	38.26
٦(MOTA	373			В	538	-16.562	1.707 22 1 00	25.18
	ATOM	373		ASP	В	538	-12.447		26.41
	MOTA	374	_	ASP		538	-12.120	2.020 == 2.00	20.76
	ATOM	374		LEU			-11.637	, 2.505 2012	19.65
_		374		LEU			-10.312		17.48
5		374		LEU			-9.56		16.46
	ATOM		_	LEU			-8.11		16.43
	ATOM						-8.05		15.57
	ATOM						-7.56	4 3.569 26.895 1.00	16.75
_	ATOM			LEU			-9.48		20.36
6	MOTA 0		-	LE			-8.86	2 2.716 22.249 1.00	20.36
	MOTA	374	.0 0	، دد د	-				

5	ATOM	3749	N	LEU	В	540	-9.487	0.803 23.239	1.00	18.23
3	ATOM	3750	CA	LEU	В	540	-8.743	-0.048 22.319	1.00	18.05
	ATOM	3751	CB	LEU	В	540	-8.909	-1.528 22.701	1.00	16.38
	ATOM	3752	CG	LEU	В	540	-8.188	-2.554 21.821	1.00	19.81
	ATOM	3753	CD1	LEU	В	540	-6.679	-2.303 21.828	1.00	19.27
10	ATOM	3754	CD2	LEU	В	540	-8.473	-3.952 22.327	1.00	18.00
10	ATOM	3755	C	LEU	В	540	-9.241	0.169 20.891	1.00	21.50
	ATOM	3756	0	LEU	В	540	-8.449	0.293 19.964	1.00	20.41
	MOTA	3757	И	LEU	В	541	-10.559	0.206 20.726	1.00	22.40
	ATOM	3758	CA	LEU	В	541	-11.164	0.419 19.413	1.00	23.27
15	MOTA	3759	CB	LEU	В	541	-12.686	0.429 19.527	1.00	25.12
13	ATOM	3760	CG	LEU	В	541	-13.410	-0.808 18.999	1.00	36.53
	ATOM	3761	CD1	LEU	В	541	-14.910	-0.671 19.273	1.00	30.98
	ATOM	3762	CD2	LEU	В	541	-13.136	-0.971 17.508	1.00	31.93
	ATOM	3763	CDZ	LEU	В	541	-10.697	1.751 18.842	1.00	22.46
20	ATOM	3764	0	LEU	В	541	-10.359	1.845 17.666	1.00	26.29
20	ATOM	3765	N	GLU	В	542	-10.694	2.781 19.680	1.00	23.96
	ATOM	3766	CA	GLU	В	542	-10.248	4.106 19.270	1.00	26.91
	ATOM	3767	CB	GLU	В	542	-10.250	5.050 20.468	1.00	30.84
	ATOM	3768	CG	GLU	В	542	-11.166	6.245 20.347	1.00	37.20
25	ATOM	3769	CD	GFA	В	542	-11.138	7.105 21.597	1.00	39.98
23	ATOM	3770	OE1	GLU	В	542	-12.223	7.385 22.144	1.00	39.92
	ATOM	3771	OE2	GLU	В	542	-10.028	7.494 22.034	1.00	38.96
	ATOM	3772	C	GLU	В	542	-8.826	4.010 18.724	1.00	27.90
	ATOM	3773	0	GLU	В	542	-8.530	4.492 17.634	1.00	29.32
30	ATOM	3774	N	MET	В	543	-7.945	3.388 19.499	1.00	26.41
20	ATOM	3775	CA	MET	В	543	-6.552	3.237 19.107	1.00	23.53
	ATOM	3776	CB	MET	В	543	-5.749	2.591 20.247	1.00	24.60
	ATOM	3777	CG	MET	В	543	-5.812	3.338 21.579	1.00	26.46
	ATOM	3778	SD	MET	В	543	-5.373	5.084 21.467	1.00	29.45
35	ATOM	3779	CE	MET	В	543	-3.585	4.971 21.349	1.00	25.43
	ATOM	3780	C	MET	В	543	-6.403	2.407 17.832	1.00	25.80
	ATOM	3781	Ō	MET	В	543	-5.535	2.686 17.004	1.00	23.59
	ATOM	3782	N	LEU	В	544	-7.254	1.394 17.673	1.00	27.74
	ATOM	3783	CA	LEU	В	544	-7.202	0.522 16.499	1.00	26.32
40	MOTA	3784	CB	LEU	В	544	-8.069	-0.721 16.719	1.00	26.75
	ATOM	3785	CG	LEÚ	В	544	-8.274	-1.632 15.502	1.00	28.12
	ATOM	3786	CD1	LEU	В	544	-6.956	-2.294 15.136	1.00	26.36
	ATOM	3787	CD2	LEU	В	544	-9.330	-2.680 15.803	1.00	27.00
	MOTA	3788	С	LEU	В	544	-7.672	1.252 15.250	1.00	26.97
45	ATOM	3789	0	LEU	В	544	-7.036	1.181 14.195	1.00	24.25
	ATOM	3790	N	ASP	В	545	-8.787	1.961 15.372	1.00	30.37
	ATOM	3791	CA	ASP	В	545	-9.338	2.702 14.244	1.00	32.34
	ATOM	3792	CB	ASP	В	545	-10.668	3.346 14.637	1.00	36.61
	MOTA	3793	CG	ASP	В	545	-11.818	2.370 14.565	1.00	42.73
50	ATOM	3794	OD1	ASP	В	545	-12.858	2.624 15.211	1.00	47.39
	ATOM	3795	OD2	ASP	В	545	-11.676	1.342 13.863	1.00	46.96
	ATOM	3796	C	ASP	В	545	-8.382	3.762 13.711	1.00	31.27
	MOTA	3797	0	ASP	В	545	-8.443	4.120 12.532	1.00	30.53
	MOTA	3798	N	ALA	В	546	-7.506	4.272 14.572	1.00	29.02
55	ATOM	3799	CA	ALA	В	546	-6.543	5.280 14.141	1.00	31.21
	MOTA	3800	CB	ALA	В	546	-5.646	5.693 15.306	1.00	30.98
	ATOM	3801	С	ALA	В	546	-5.697	4.731 12.996	1.00	32.14
	ATOM	3802	0	ALA	В	546	-5.189	5.490 12.170	1.00	33.78
	ATOM	3803	N	HIS	В	547	~5.555	3.410 12.943	1.00	32.27
60	MOTA	3804	CA	HIS	В	547	-4.773	2.767 11.892	1.00	37.73
	MOTA	3805	CB	HIS	В	547	-3.991	1.576 12.457	1.00	35.83

5	ATOM	3806	CG	HIS	В	547	-2.796		13.269	1.00	34.54
,	ATOM		CD2	HIS	В	547	-2.698		14.486	1.00	30.23
	ATOM		ND1	HIS	В	547	-1.502		12.840	1.00	34.23
	MOTA		CE1	HIS	В	547	-0.659		13.760	1.00	36.72 31.48
	ATOM	3810	NE2	HIS	В	547	-1.360		14.768	1.00	43.69
10	ATOM	3811	C	HIS	В	547	-5.649		10.735	1.00	46.04
	ATOM	3812	0	HIS	В	547	-5.178	2.152	9.606	1.00	48.35
	MOTA	3813	N	ARG	В	548	-6.919		11.019	1.00	54.74
	ATOM	3814	CA	ARG	В	548	-7.843	1.551	9.993	1.00	54.66
	ATOM	3815	CB	ARG	В	548	-8.522		10.452 9.681	1.00	59.94
15	MOTA	3816	С	ARG	В	548	-8.886	2.619		1.00	62.81
	ATOM	3817	0	ARG	В	548	-8.580	3.812		1.00	64.81
	ATOM	3818	N	LEU	В	549	-10.116	2.186 3.109		1.00	67.59
	MOTA	3819	CA	LEU	В	549	-11.204	2.327		1.00	68.06
	MOTA	3820	CB	LEU	В	549	-12.478		10.275	1.00	69.12
20	MOTA	3821	С	LEU	В	549	-11.449		10.275	1.00	68.96
	MOTA	3822	0	LEU	В	549	-11.451		11.412	1.00	70.70
	MOTA	3823	OXT	LEU	В	549	-11.634 -4.547		22.000	1.00	18.55
	HETATM	3824	CP9	DES	В	600	-3.163		21.467	1.00	17.72
	HETATM	3825	CP8	DES	В	600	-2.897		21.381	1.00	21.17
25	HETATM	3826	CP7	DES	В	600	-3.719		20.374	1.00	22.05
	HETATM	3827	CP6	DES	В	600 600	-3.405		18.998	1.00	21.32
	HETATM	3828	CP1	DES	В	600	-4.239		18.063	1.00	21.61
	HETATM	3829	CP2	DES	В	600	-5.388		18.509	1.00	24.89
••	HETATM	3830	CP3	DES	B B	600	-6.244		17.600	1.00	24.94
30	HETATM	3831	OP3	DES DES	В	600	-5.718		3 19.860	1.00	24.08
	HETATM	3832	CP4	DES	В	600	-4.877		20.791	1.00	24.67
	HETATM	3833	CP5 C7	DES	В	600	-1.998		22.190	1.00	16.67
	HETATM	3834 3835	C6	DES	В	600	-1.330	-7.834	4 23.325	1.00	15.39
25	HETATM	3836	C5	DES	В	600	-2.054	-7.643	2 24.522	1.00	17.62
35	HETATM HETATM	3837	C4	DES	В	600	-1.433		2 25.634		16.16
	HETATM	3838	C3	DES	В	600	-0.077		5 25.542		20.04
	HETATM	3839	03	DES	В	600	0.509		3 26.655		15.55
	HETATM	3840		DES	В	600	0.669		6 24.353		18.94
40	HETATM			DES	В	600	0.035		0 23.241		
70	HETATM			DES	В	600	-1.642		3 21.942		17.61
	HETATM	-		DES	В	600	-0.440		9 20.998		11.63
	HETATM			CBM	В	417	-4.997	-22.99	4 25.273	1.00	
	HETATM			CBM	В	417	-4.789	-24.18	7 25.003	1.00	
45	HETATM			CBM	B	417	-4.798	-22.55	9 26.552	1.00	
,,,	HETATM			CBM	В	417	-5.468	-21.96	0 24.264	1.00	
	HETATM			CBM	В	530	-15.278		4 10.243		
	HETATM		04	CBM	В	530	-15.852	-5.08			
	HETATM			CBM	В	530	-15.832		1 11.201		
50	HETATM			CBM	В	530	-14.207		6 10.628		
	MOTA	3852	CB	HIS	C	687	9.818		0 -2.211		
	ATOM	3853	3 C	HIŞ		687	10.133		7 -4.689		
	MOTA	3854	1 O	HIS	С	687	11.204		0 -4.472		
	ATOM	3855	5 N	HIS		687	7.944		3 -3.758		
55		3856	CA	HIS		687	9.424		4 -3.586		
23	ATOM	3857		LYS		688	9.533		1 -5.879		
	ATOM	3858	B CA	LYS	C	688	10.101		9 -7.00		
	ATOM	3859	9 CB	LYS		688	8.980	-21.54	0 -7.90	1 1.00 7 1.00	
	ATOM	3860	o C	LYS		688	11.050	-20.12	27 -7.82		
60		386		LYS		688	12.253	-20.3	79 -7.85		
	MOTA	386	2 N	ILE	C	689	10.511	-19.10	3 -8.48	٠ ١.٠٠	, ,,,,

-			63		_	600	11 706	10 010 0 206		F3 00
5	ATOM	3863	CA	ILE	C	689		-18.212 -9.306	1.00	53.09
	ATOM	3864	CB	ILE	C	689	10.496		1.00	53.83
	ATOM	3865	CG2	ILE	С	689	11.334		1.00	54.55
	ATOM	3866	CG1	ILE	С	689	9.229	-17.603-10.551	1.00	52.90
	ATOM	3867	CD1	ILE	C	689	8.406	-16.550-11.258	1.00	50.45
10	ATOM	3868	С	ILE	С	689	12.513	-17.611 -8.560	1.00	50.82
	MOTA	3869	0	ILE	С	689	13.616	-17.550 -9.097	1.00	51.28
	MOTA	3870	N	LEU	C	690	12.288	-17.162 -7.329	1.00	48.01
	ATOM	3871	CA	LEU	C	690	13.362	-16.570 -6.534	1.00	47.33
	ATOM	3872	CB	LEU	С	690	12.812	-16.058 -5.199	1.00	42.51
15	ATOM	3873	CG	LEU	С	690	13.835	-15.501 -4.206	1.00	40.67
	ATOM	3874	CD1	LEU	С	690	14.575	-14.324 -4.831	1.00	39.95
	ATOM	3875	CD2	LEU	С	690	13.128	-15.078 -2.926	1.00	38.77
	ATOM	3876	С	LEU	C	690	14.445	-17.615 -6.282	1.00	48.87
	ATOM	3877	0	LEU	С	690	15.643	-17.340 -6.393	1.00	46.71
20	MOTA	3878	N	HIS	C	691	14.001	-18.818 -5.939	1.00	51.36
	MOTA	3879	CA	HIS	С	691	14.886	-19.946 -5.675	1.00	53.35
	MOTA	3880	CB	HIS	С	691	14.042	-21.203 -5.460	1.00	58.64
	ATOM	3881	CG	HIS	C	691	14.655	-22.195 -4.526	1.00	62.94
	ATOM	3882	CD2	HIS	C	691	15.503	-23.227 -4.751	1.00	64.95
25	MOTA	3883	ND1	HIŞ	С	691	14.392	-22.202 -3.173	1.00	65.49
	ATOM	3884	CEl	HIS	С	691	15.053	-23.195 -2.605	1.00	68.18
	MOTA	3885	NE2	HIS	C	691	15.733	-23.833 -3.540	1.00	68.77
	MOTA	3886	C	HIS	C	691	15.824	-20.162 -6.861	1.00	52.19
	ATOM	3887	0	HIS	C	691	17.048	-20.153 -6.717	1.00	47.53
30	MOTA	3888	N	ARG	C	692	15.222	-20.350 -8.032	1.00	52.37
	MOTA	3889	CA	ARG	С	692	15.949	-20.586 -9.271	1.00	52.90
	MOTA	3890	CB	ARG	С	692	14.955	-20.832-10.410	1.00	54.04
	MOTA	3891	CG	ARG	C	692	15.575	-20.826-11.797	1.00	57.52
	ATOM	3892	CD	ARG	C	692	14.528	-21.048-12.874	1.00	58.25
35	ATOM	3893	NE	ARG	C	692	14.375	-19.878-13.732	1.00	61.43
	MOTA	3894	CZ	ARG	C	692	13.218	-19.260-13.951	1.00	64.32
	MOTA	3895	NH1	ARG	C	692	12.108	-19.706-13.378	1.00	63.22
	MOTA	3896	NH2	ARG	C	692	13.171	-18.197-14.746	1.00	65.93
	ATOM	3897	С	ARG	C	692	16.873	-19.434 -9.639	1.00	53.09
40	MOTA	3898	0	ARG	C	692	18.047	-19.644 -9.956	1.00	53.06
	ATOM	3899	N	LEU	C	693	16.338	-18.217 -9.607	1.00	50.73
	ATOM	3900	CA	LEU	C	693	17.125	-17.039 -9.945	1.00	49.53
	ATOM	3901	CB	LEU	C	693	16.249	-15.784 -9.881	1.00	49.56
	ATOM	3902	CG	LEU	C	693		-15.245-11.239	1.00	49.78
45	ATOM	3903	CD1	LEU	C	693		-16.389-12.079	1.00	50.30
	ATOM	3904	CD2	LEU	C	693		-14.170-11.037	1.00	48.79
	ATOM	3905	С	LEU	C	693	18.318	-16.904 -9.006	1.00	48.38
	ATOM	3906	0	LEU	C	693	19.382	-16.426 -9.402	1.00	46.35
	ATOM	3907	N	LEU	C	694	18.135	-17.329 -7.761	1.00	46.74
50	ATOM	3908	CA	LEU	C	694	19.204		1.00	49.41
	ATOM	3909	CB	LEU	C	694		-17.415 -5.362	1.00	45.20
	ATOM	3910	CG	LEU	C	694	18.222	-16.128 -4.643	1.00	40.19
	MOTA	3911	CD1	LEU	С	694		-16.474 -3.371	1.00	41.65
	MOTA	3912	CD2	LEU	C	694	19.453	-15.307 -4.317	1.00	35.91
55	ATOM	3913	С	LEÙ	C	694		-18.417 -7.058	1.00	54.15
	ATOM	3914	0	LEU	С	694		-18.320 -6.776	1.00	53.55
	ATOM	3915	N	GLŅ	C	695		-19.498 -7.619	1.00	57.44
	ATOM	3916	CA	GLN	C	695			1.00	62.46
_	ATOM	3917	CB	GLN	C	695	19.477	-21.853 -8.304	1.00	61.95
60	MOTA	3918	CG	GLN	С	695	19.548	-23.010 -7.311	1.00	61.49
	ATOM	3919	CD	GLN	С	695	18.454	-24.053 -7.490	1.00	62.78

								-24.928 -	6 653	1.00	63.33
5	ATOM		OE1		С	695		-24.928 - -23.969 -			60.37
	MOTA		NE2		C	695		-23.905 -20.414 -			65.13
	MOTA		C		С	695		-20.414 -20.740 -			65.87
	MOTA	3923	0		C	695		-20.740 -19.824-1			67.67
	ATOM	3924	N		C	696		-19.500-1	-	1.00	70.66
10	MOTA	3925	CA	ASP	С	696		-19.300-1	_	1.00	71.06
	ATOM	3926	CB	ASP	C	696		-18.346-1 -18.792-1		1.00	71.70
	MOTA	3927	CG	ASP	C	696	= 1	-18.752-3 -18.455-3	14 521	1.00	72.47
	MOTA	3928	OD1	ASP	С	696		-18.455-	13.321	1.00	71.41
	MOTA	3929	OD2	ASP	C	696		-19.478-		1.00	72.41
15	MOTA	3930	С	ASP	С	696	22.951	-19.132-		1.00	72.56
	ATOM	3931	0	ASP	C	696	23.245	-19.967-		1.00	74.67
	MOTA	3932	N	SER	С	697	23.859	-19.741-		1.00	76.45
	MOTA	3933	CA	SER	С	697	25.291	-19.741-		1.00	76.00
	ATOM	3934	CB	SER	С	697	26.019	-18.960-		1.00	78.44
20	MOTA	3935	С	SER	С	697	25.841	-18.960-		1.00	79.20
	MOTA	3936	0	SER	С	697	26.286	-17.809-		1.00	80.07
	ATOM	3937	OXT	SER	С	697	25.818	13.661		1.00	50.28
	ATOM	3938	CB	LYS	D	686	-14.070	14.418		1.00	51.59
	MOTA	3939	С	LYS	D	686	-13.682	14.418		1.00	50.42
25	MOTA	3940	0	LYS	D	686	-12.629	15.796		1.00	50.43
	MOTA	3941	N	LYS	D	686	-12.910	14.872		1.00	50.62
	MOTA	3942	CA	LYŚ	D	686	-13.976	13.676		1.00	49.91
	MOTA	3943	N	HIS	Ď	687	-14.617	13.076		1.00	51.28
	ATOM	3944	CA	HIS	D	687	-14.447	12.984	21.144	1.00	54.12
30	MOTA	3945		HIS	D	687	-15.806	12.336		1.00	60.06
	MOTA	3946		HIS	D	687	-15.713			1.00	61.05
	MOTA	3947		HIS	D	687	-15.418			1.00	62.39
	ATOM	3948		HIŞ	D	687	-15.911		25.378	1.00	62.76
	MOTA	3949		HIS	D	687	-15.741		24.912	1.00	63.46
35	MOTA	3950		HIS	D	687	-15.441	_		1.00	49.55
	MOTA	3951		HIS	D	687	-13.691 -14.099		20.524	1.00	50.84
	MOTA	3952		HIS	D	687	-12.593		21.909	1.00	44.00
	MOTA	3953		LYS	D	688	-12.593		22.038	1.00	40.31
	MOTA	3954		LYS	D	688	-10.446		21.299	1.00	41.42
40	MOTA	3955		LYS	D	688	-10.440		19.780	1.00	42.76
	MOTA	3956		LYS	D	688	-9.123		19.152	1.00	38.66
	MOTA	395		LYS	D	688	-9.123 -9.162		17.640	1.00	
	MOTA		B CE	LYS	D	688	-7.894		16.986	1.00	
	MOTA	395		LYS	D	688 688	-11.506		23.517	1.00	36.70
45	ATOM	396		LYŞ	D		-11.27		24.266	1.00	33.38
	ATOM	396		LYS	D	688	-11.549		23.942	1.00	33.06
	MOTA	396		ILE	D	689 689	-11.25		25.328		28.70
	MOTA	396		ILE	D	689	-11.438		25.607		30.88
	MOTA	396		ILE	D	689	-10.72		26.899		31.45
50		396			D	689	-12.92		25.721	1.00	32.57
	ATOM	396			D		-13.30		25.031		
	MOTA	396			D	689			25.541		
	MOTA	396		ILE		689	-9.79 -9.40		26.611		
	MOTA	396		ILE			-8.98		24.496		
55		397		LEU			-8.98 -7.56		24.549		
	MOTA	397		LEU			-7.56 -6.90		23.200		
	MOTA	397		LEU					7 22.992		_
	MOTA	397		LEU			-5.43 -4.59		24.108		
	MOTA	397					-4.59 -4.95		3 21.616		
60		397					-4.95 -7.34		3 24.902		
	ATOM	397	76 C	LEU	ם ז	690	-7.54				

5	ATOM	3977	0	LEU	D	690	-6.408	11.165 25.625	1.00	28.34
	ATOM	3978	N	HIS	D	691	-8.206	11.694 24.383		
	ATOM	3979	CA	HIS	D	691	-8.107	13.125 24.665		
	ATOM	3980		HIS	D	691	-9.156	13.907 23.861		
	ATOM	3981	CG	HIS	D	691	-8.903	13.935 22.386		
10	ATOM	3982	CD2	HIS	D	691	-7.750	14.000 21.679		
	MOTA	3983	ND1	HIS	D	691	-9.920			
	ATOM	3984		HIS	D	691		13.906 21.458	1.00	
	ATOM	3985	NE2	HIS	D		-9.407	13.953 20.242	1.00	
	ATOM	3986	C			691	-8.091	14.010 20.347	1.00	
15	ATOM	3987	0	HIS	D	691	-8.338	13.373 26.159	1.00	
	ATOM	3988		HIS	D	691	-7.602	14.120 26.802	1.00	
	ATOM		N	ARG	D	692	-9.371	12.742 26.703	1.00	
		3989	CA	ARG	D	692	-9.691	12.912 28.114	1.00	29.11
	ATOM	3990	CB	ARG	D	692	-10.959	12.134 28.472	1.00	30.84
20	ATOM	3991	CG	ARG	D	692	-11.255	12.129 29.963	1.00	41.63
20	ATOM	3992	CD	ARG	D	692	-12.502	11.327 30.290	1.00	48.83
	ATOM	3993	NE	ARG	D	692	-13.618	12.198 30.647	1.00	54.50
	ATOM	3994	CZ	ARG	D	692	-14.498	12.677 29.774	1.00	59.37
	ATOM	3995	NH1	ARG	D	692	-14.392	12.371 28.486	1.00	60.97
2.5	MOTA	3996	NH2	ARG	D	692	-15.483	13.464 30.188	1.00	59.07
25	ATOM	3997	С	ARG	D	692	-8.548	12.451 29.011	1.00	28.30
	ATOM	3998	0	ARG	D	692	-8.139	13.167 29.929	1.00	26.50
	MOTA	3999	N	LEU	D	693	-8.030	11.259 28.737	1.00	24.87
	ATOM	4000	CA	LEU	D	693	-6.943	10.705 29.536	1.00	27.17
• •	ATOM	4001	CB	LEU	D	693	-6.674	9.254 29.116	1.00	28.45
30	ATOM	4002	CG	LEU	D	693	-7.844	8.300 29.391	1.00	30.40
	ATOM	4003	CD1	LEU	D	693	-7.575	6.932 28.778	1.00	34.79
	MOTA	4004	CD2	LEU	D	693	-8.043	8.171 30.894	1.00	32.02
	ATOM	4005	C	LEU	D	693	-5.670	11.539 29.440	1.00	25.96
	MOTA	4006	0	LEU	D	693	-4.948	11.700 30.428	1.00	27.01
35	MOTA	4007	N	LEU	D	694	-5.395	12.080 28.257	1.00	25.33
	ATOM	4008	CA	LEU	D	694	-4.207	12.906 28.062	1.00	27.22
	ATOM	4009	CB	LEU	D	694	-3.948	13.126 26.572	1.00	
	MOTA	4010	CG	LEU	D	694	-3.118	12.080 25.825	1.00	24.61
	ATOM	4011	CD1	LEU	D	694	-3.230	12.332 24.324		22.20
40	ATOM	4012	CD2	LEU	D	694	-1.666	12.148 26.275	1.00	21.13
	ATOM	4013	С	LEU	D	694	-4.336	14.270 28.742	1.00	21.34
	MOTA	4014	0	LEU	D	694	-3.339	14.889 29.102	1.00	32.40
	ATOM	4015	N	GLN	D	695	-5.570	14.733 28.915	1.00	31.55
	ATOM	4016	CA	GLN	D	695	-5.820	16.032 29.528	1.00	36.93
45	ATOM	4017	CB	GLN	D	695	-7.022		1.00	43.18
	ATOM	4018	CG	GLN	D	695	-6.772	16.694 28.862	1.00	40.48
	ATOM	4019	CD	GLN	D	695	-7.943	17.071 27.422	1.00	37.99
	ATOM	4020	OE1	GLN	D	695		17.764 26.795	1.00	35.86
	ATOM	4021	NE2	GLN	D	695	-7.863	18.895 26.342	1.00	38.84
50	ATOM	4022	C	GLN	D	695	-9.082	17.060 26.757	1.00	31.62
	ATOM	4023	0	GLN			-6.049	16.009 31.034	1.00	48.74
	ATOM	4024	N		D	695	-6.119	17.065 31.660	1.00	51.25
	ATOM	4025	CA	ASP	D	696	-6.175	14.818 31.611	1.00	54.01
	ATOM	4025		ASP	D	696	-6.398	14.702 33.047	1.00	62.23
55	ATOM	4026	CB	ASP	D	696	-6.217	13.238 33.485	1.00	63.97
23	ATOM		CG	ASP	D	696	-7.527	12.467 33.475	1.00	67.72
		4028	OD1	ASP	D	696	-8.528	12.996 32.941	1.00	68.11
	ATOM	4029	OD2	ASP	D	696	-7.552	11.333 34.003	1.00	68.95
	ATOM	4030	C	ASP	D	696	-5.456	15.622 33.840	1.00	65.60
60	ATOM	4031	0	ASP	D	696	-4.312	15.189 34.134	1.00	68.33
υŪ	ATOM	4032	OXT	ASP	D	696	-5.874	16.755 34.140	1.00	69.20
	HETATM	4033	0	нон		1	16.153	-0.605 -4.425	1.00	17.11

			_	*****	2	16.570	-5.304-16.560	1.00	21.44
5	HETATM	4034	0	нон	3	18.526	0.742 -4.495	1.00	23.43
	HETATM	4035		нон	4	13.647	-2.187 8.588	1.00	25.82
	HETATM	4036	0	нон		9.778	-5.825 2.509	1.00	20.58
	HETATM	4037	0	нон	5 6	17.072	-3.605 -8.015	1.00	18.38
	HETATM	4038	0	нон	7	24.920	-1.689 -2.780		25.74
10	HETATM	4039	0	нон		7.321	-5.649 5.061		24.11
	HETATM	4040	0	нон	8	25.976	-3.535 15.158		26.78
	HETATM	4041	0	нон	9		-7.006-15.192		19.64
	HETATM	4042	0	нон	10	15.088	0.925 -5.953		20.55
	HETATM	4043	0	HOH	11	14.070	3.407 -6.654	1.00	32.30
15	HETATM	4044	0	нон	12	18.008	-8.393 13.487	1.00	30.64
	HETATM	4045	0	нон	13	31.949	-2.804 -4.279	1.00	24.45
	HETATM	4046	0	нон	14	19.625	1.079-21.140	1.00	25.87
	HETATM	4047	0	нон	15	11.741	13.951 14.153	1.00	31.07
	HETATM	4048	0	нон	16	25.067	1.323-10.393	1.00	21.01
20	HETATM	4049	0	HOH	17	15.501	3.349-11.482	1.00	24.28
	HETATM	4050	0	нон	18	13.880	0.979 -8.828	1.00	35.26
	HETATM	4051	0	нон	19	17.591	-2.041 -0.314	1.00	37.90
	HETATM	4052	0	нон	20	23.682	9.496 11.841	1.00	39.44
	HETATM	4053	0	HOH	21	15.754	7.574 -3.066	1.00	37.67
25	HETATM	4054	0	нон	22	-4.943	0.354-15.982		36.92
	HETATM	4055	0	нон	23	6.877	-4.002 8.671	1.00	30.38
	HETATM	4056	0	HOH	24	15.806	-3.158 -5.321		28.89
	HETATM	4057		нон	25	17.185	9.249 17.009		30.15
	HETATM	4058		нон	26	17.572	-2.929 11.604		31.37
30	HETATM	4059		HOH	27	24.096	-5.871-11.980		32.74
	HETATM	4060		HOH	28	22.324	-12.361 -0.801		36.61
	HETATM	4061		HOH	29	27.547	13.442 -2.719		35.41
	HETATM	4062	2 0	нон	30	11.173	-9.527 5.483		29.88
	HETATM	4063		HOH	31	15.438	-6.564 5.983		35.05
35	HETATM	4064	10	нон	32	9.946	11.680-15.263		38.68
	HETATM	4065		нон	33	7.599	10.503 -5.109		42.66
	HETATM	4066	5 0	HOH	34	20.112	10.343 14.897		41.73
	HETATM	406	7 0	HOH	35	15.972	-5.914 -9.527		28.08
	HETATM	406		нон	36	22.401	-0.899 -8.109		33.13
40	HETATM	406		нон	37	16.128	15.655 -3.706		41.37
	HETATM	407		HOH	38	3.581	13.545 21.339		37.79
	HETATM	407		нон	39	31.900	-7.530 14.119		47.51
	HETATM	407	2 0	нон	40	20.058	6.668 15.63		29.24
	HETATM	407		нон	41	34.634	10.511 -9.08	5 1.00	44.60
45	HETATM	407		нон	42	17.968	-17.325 -4.08		44.10
	HETATM			HOH	43	23.258			15.22
	HETATM	407	6 0	нон	44	4.034	-0.018 36.08		21.11
	HETATM	407	7 0	нон	45	-5.943			19.51
	HETATM	407	8 0	нон	46	6.084			27.74
50	HETATM			нон	47	9.762			
	HETATM	408	0 0	нон	48	1.804			
	HETATM	408	1 0	нон	49	0.929			
	HETATM	408	2 0	нон	50	9.627			
	HETATM	408	3 0	HOH	51	2.121			
55			34 0	HOH	52	20.060			
	HETATM		35 0	нон	53	-6.786			
	HETATM	1 408	36 0	нон	54	2.751			
	HETATM	1 408	37 0	нон	55	5.994			
	HETATM	408	88 0	нон	56	19.416			
60	HETATN				57	4.833			
	HETAT	409	90 0	нон	58	-7.638	8 -8.931 37.80	,, 1.00	,,

5	HETATM	4091	0	нон	59	28.442	-4.673 21.875	1.00	24.32
	HETATM	4092	0	нон	60	1.094	-4.893 32.100	1.00	24.27
	HETATM	4093	0	нон	61	0.905	-7.306 32.783	1.00	21.33
	HETATM	4094	0	НОН	62	3.396	-2.971 32.306	1.00	26.13
	HETATM	4095	0	нон	63	10.363	4.576 28.391	1.00	33.43
10	HETATM	4096	0	НОН	64	19.551	-6.473 16.597	1.00	35.38
-	HETATM	4097	ō	НОН	65	-2.888	-19.627 15.665	1.00	27.99
	HETATM	4098	ō	НОН	66	-7.275	-9.745 31.077	1.00	27.00
	HETATM	4099	ō	нон	67	10.189	3.580 16.510	1.00	24.19
	HETATM	4100	ō	нон	6.8	2.741	0.716 28.382	1.00	16.48
15	HETATM	4101	Ö	нон	69	23.522	-4.323 13.943	1.00	27.48
	HETATM	4102	Ö	нон	70	17.133	8.133 19.686	1.00	32.24
	HETATM	4103	o	нон	71	-0.295	4.535 35.884	1.00	33.42
	HETATM	4104	0	нон	72	9.519	10.828 34.842	1.00	29.38
	HETATM	4105	o	нон	73	6.291	14.878 29.070	1.00	28.21
20	HETATM	4106	Ö	нон	74	-1.721	6.480 13.381	1.00	49.91
	HETATM	4107	Ö	нон	75	10.091	-15.427 26.194	1.00	24.17
	HETATM	4108	o	нон	76	5.029	7.461 17.718	1.00	18.91
	HETATM	4109	o	нон	77	3.758	2.086 14.306	1.00	28.28
	HETATM	4110	o	нон	78	-1.390	-18.739 33.183	1.00	41.11
25	HETATM	4111	Ö	нон	79	12.703	-8.687 32.119	1.00	36.21
	HETATM	4112	Ö	нон	80	22.270	-6.451 14.844	1.00	33.21
	HETATM	4113	Ö	нон	81	1.458	4.605 34.026	1.00	23.59
	HETATM	4114	Ö	нон	82	1.759	-2.158 30.374	1.00	28.78
	HETATM	4115	Ö	нон	83	6.153	-21.372 23.188	1.00	31.14
30	HETATM	4116	ō	нон	84	36.525	0.463 20.792	1.00	45.26
	HETATM	4117	ō	нон	85	13.832	9.696 13.792	1.00	33.12
	HETATM	4118	0	нон	86	31.166	6.635 24.924	1.00	35.19
	HETATM	4119	Ô	нон	8.7	8.844	-10.389 34.180	1.00	48.80
	HETATM	4120	0	нон	88	9.581	-6.956 34.136	1.00	42.95
35	HETATM	4121	0	НОН	89	-1.563	15.887 27.596	1.00	39.35
	HETATM	4122	0	нон	90	-5.286	10.345 32.757	1.00	35.20
	HETATM	4123	0	нон	91	15.035	0.607 13.339	1.00	29.53
	HETATM	4124	0	HOH	92	-10.984	-1.500 30.272	1.00	29.84
	HETATM	4125	0	нон	93	-7.239	-0.271 -1.207	1.00	48.98
40	HETATM	4126	0	нон	94	18.022	-4.902 34.286	1.00	35.28
	HETATM	4127	0	нон	95	29.347	-6.319 19.920	1.00	37.20
	HETATM	4128	0	нон	96	-14.309	-19.369 20.945	1.00	30.23
	HETATM	4129	0	нон	97	31.496	4.614 18.716	1.00	38.79
	HETATM	4130	0	НОН	98	26.567	9.759 25.629	1.00	29.72
45	HETATM	4131	0	НОН	99	2.848	14.531 1.134	1.00	38.08
	HETATM	4132	0	нон	100	-9.373	5.699 -7.953	1.00	53.23
	HETATM	4133	0	нон	101	-10.137	-0.553 -6.742	1.00	47.72
	HETATM	4134	0	нон	102	10.558	-10.363 15.403	1.00	40.97
	HETATM	4135	0	нон	103	21.079	17.166 18.929	1.00	32.40
50	HETATM	4136	0	нон	104	25.810	-5.921 22.506	1.00	37.69
	HETATM	4137	0	нон	105	22.493	-1.311 34.465	1.00	49.94
	HETATM	4138	0	нон	106	19.317	10.977 38.703	1.00	40.60
	HETATM	4139	0	нон	107	4.479	13.951 3.045	1.00	45.33
	HETATM	4140	0	нон	108	20.418	19.353 34.044	1.00	42.18
55	HETATM	4141	0	нон	109	-3.065	8.936 14.062	1.00	38.41
	HETATM	4142	0	нон	110	26.856	-4.674-10.940	1.00	55.67
	HETATM	4143	0	нон	111	2.032	-6.387 5.614	1.00	42.23
	HETATM	4144	0	нон	112	0.601	0.228-17.268	1.00	40.57
	HETATM	4145	0	нон	113	4.903	13.488-14.050	1.00	47.72
60	HETATM	4146	0	нон	114	3.986	16.140 -0.960	1.00	40.66
	HETATM	4147	0	нон	115	12.968	-19.561 2.741	1.00	40.76

5 10 15 20 25	HETATM	4148 4149 4150 4151 4153 4154 4155 4155 4157 4158 4161 4162 4163 4164 4165 4166 4167 417 417 417 417		HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH	116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141	21.728 31.650 25.421 10.317 22.723 6.702 27.987 30.798 10.071 9.562 6.712 5.927 4.472 6.792 24.513 -2.528 -7.864 11.577	-24.786 22.178 -7.370 10.436 -9.457 14.887 9.556 13.557 16.499 -0.571 8.334 6.058 8.454 6.306 7.721 11.582 -20.363 7.706 -16.962	20.174 26.686 28.325 31.983 21.642 21.161 12.998 15.427 37.596 7.167 7.588 -20.393 -21.392 8.822 10.594 510.973 7.051 23.724 12.354 519.248 24.398		39.43 33.36
30 35	HETATM HETATM HETATM	4177 4177 4177 4177 4177 4177 4177	L 0 2 0 3 0 4 0 5 0 6 0 7 0	нон нон	139 140	-2.528 -7.864	-20.361 7.706 -16.962 12.263 -14.19 -16.70 -20.10	L 12.354 5 19.248	1.00 1.00 1.00 1.00 1.00 1.00	52.13 47.82 39.43 33.36 51.32 57.11 43.01 49.96

5

Appendix 3

Atomic Coordinates for Human ERa Complexed With OHT

10	CRYST1	58.24	12 58.:	242	277.46	90.00	90.00	120.00	P 65	2 2	12
	ORIGX1	1.0	00000	0.00	0000	0.000000	0.00	000			
	ORIGX2		00000	1.00	0000	0.000000					
	ORIGX3	0.0	00000	0.00	0000	1.000000	0.00	000			
	SCALE1	0.0	17170	0.00	9913	0.000000	0.00	000			
15	SCALE2	0.0	00000	0.01	9826	0.00000	0.00	000			
	SCALE3	0.0	00000	0.00	0000	0.003604	0.00	000			
	MOTA	1	CB	LEU	306	6.638	11.502		1.00	61.	
20	ATOM	2	C	LEU	306	7.381	10.684		1.00	61.	
20	ATOM	3	O	LEU	306	6.407	11.020		1.00	62.	
	ATOM ATOM	4 5	N CA	LEU LEU	306 306	6.369	9.128		1.00	62. 61.	
	ATOM	6	N N	ALA	306	7.232 8.609	10.330		1.00	60.	
	ATOM	7	CA	ALA	307	8.891	10.803		1.00	58.	
25	ATOM	8	CB	ALA	307	10.318	10.512		1.00	59.	
20	ATOM	9	C	ALA	307	8.692	12.393		1.00	57.	
	MOTA	10	Ö	ALA	307	8.451	12.770		1.00		
	ATOM	11	N	LEU	308	8.789	13.228		1.00		
	ATOM	12	CA	LEU	308	8.638	14.668		1.00		
30	ATOM	13	CB	LEU	308	9.298	15.402		1.00		
	ATOM	14	CG	LEU	308	10.637	14.822		1.00		
	MOTA	15	CD1	LEU	308	10.474	14.189		1.00		
	ATOM	16	CD2	LEU	308	11.694	15.920	5.933	1.00	58.	46
	ATOM	17	С	LEU	308	7.190	15.130	7.710	1.00	56.	51
35	ATOM	18	0	LEU	308	6.935	16.307	7.961	1.00	5 5 .	58
	MOTA	19	N	SER	309	6.246	14.208	7.546	1.00	57.	04
	ATOM	20	CA	SER	309	4.828	14.544	7.657	1.00		
	ATOM	21	CB	SER	309	4.034	13.896	6.514	1.00		
4.0	ATOM	22	OG	SER	309	4.071	12.479		1.00		
40	ATOM	23	С	SER	309	4.261	14.095		1.00		
	ATOM	24	0	SER	309	3.166	14.507		1.00		
	ATOM	25	N	LEU	310	5.016	13.257		1.00		
	ATOM	26	CA	LEU	310	4.591	12.749		1.00		
45	ATOM ATOM	27	CB	LEU	310	5.651	11.811		1.00		
43	ATOM	28 29	CG CD1	LEU LEU	310 310	5.586 5.530	10.333		1.00		
	ATOM	30	CD1	LEU	310	6.809	9.610		1.00		
	ATOM	31	CD2	LEU	310	4.330	13.865		1.00		
	ATOM	32	0	LEU	310	4.330	14.905		1.00		
50	ATOM	33	N	THR	311	3.352	13.641		1.00		
	ATOM	34	CA	THR	311	3.017	14.604		1.00		
	ATOM	35	CB	THR	311	1.527	14.554		1.00		
	ATOM	36	OG1	THR	311	1.242	13.311	•	1.00		
	ATOM	37	CG2	THR	311	0.666	14.688		1.00		
55	ATOM	38	C	THR	311	3.815	14.201		1.00		
	ATOM	39	Ö	THR	311	4.371	13.103		1.00		
	ATOM	40	N	ALA	312	3.857	15.078		1.00		
	ATOM	41	CA	ALA	312	4.590	14.798		1.00		
	ATOM	42	CB	ALA	312	4.359	15.910		1.00		
60	ATOM	43	С	ALA	312	4.171	13.460		1.00		

5	ATOM	44	0	ALA	312	5.009	12.609	18.262	1.00	45.52
ر		45	И	ASP	313	2.868	13.275	18.143	1.00	47.58
	ATOM		CA	ASP	313	2.367	12.032	18.714	1.00	47.63
	ATOM	46	CB	ASP	313	0.848	12.100	18.879	1.00	51.96
	ATOM	47	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
10	ATOM	48			313	1.314	13.234	20.929	1.00	56.38
10	ATOM	49	OD1	ASP	313	-0.785	13.117	20.282	1.00	59.15
	MOTA	50	OD2	ASP		2.745	10.846	17.835	1.00	43.93
	ATOM	51	С	ASP	313	2.745	9.741	18.330	1.00	44.77
	ATOM	52	0	ASP	313		11.081	16.531	1.00	44.52
	MOTA	53	N	GLN	314	2.826 3.182	10.028	15.588	1.00	44.73
15	MOTA	54	CA	GLN	314		10.028	14.156	1.00	45.05
	MOTA	55	CB	GLN	314	2.849	9.886	13.626	1.00	48.47
	MOTA	56	CG	GLN	314	1.534	10.646	12.428	1.00	50.37
	MOTA	57	CD	GLN	314	0.982		11.856	1.00	49.38
	MOTA	58	OEl	GLN	314	1.649	11.515	12.043	1.00	51.74
20	ATOM	59	NE2	GLN	314	-0.248	10.318 9.722	15.707	1.00	43.26
	MOTA	60	С	GLN	314	4.673		15.555	1.00	43.93
	MOTA	61	0	GLN	314	5.100	8.580	15.980	1.00	42.29
	MOTA	62	N	MET	315	5.459	10.757	16.130	1.00	41.26
	MOTA	63	CA	MET	315	6.901	10.606		1.00	42.43
25	MOTA	64	CB	MET	315	7.565	11.985	16.224	1.00	42.34
	ATOM	65	CG	MET	315	9.082	11.939	16.356	1.00	46.22
	MOTA	66	SD	MET	315	9.906	11.190	14.925 13.680	1.00	37.32
	MOTA	67	CE	MET	315	9.547	12.408	17.379	1.00	38.89
	MOTA	68	C	MET	315	7.218	9.791	17.335	1.00	40.02
30	MOTA	69	0	MET	315	8.002	8.841		1.00	37.65
	MOTA	70	N	LAV	316	6.599	10.165	18.491 19.756	1.00	39.56
	MOTA	71	CA	VAL	316	6.819	9.476	20.897	1.00	39.22
	MOTA	72	CB	VAL	316	6.023	10.136	20.897	1.00	44.43
	MOTA	73	CG1	VAL	316	6.245	9.373	21.059	1.00	41.04
35	MOTA	74	CG2	VAL	316	6.446	11.583	19.664	1.00	40.04
	MOTA	75	C	VAL	316	6.404	8.012	20.077	1.00	37.86
	ATOM	76	0	VAL	316	7.141	7.117	19.127	1.00	41.90
	MOTA	77	И	SER	317	5.215	7.767	18.997	1.00	41.68
	MOTA	78	CA	SER	317	4.733	6.400 6.402	18.415	1.00	43.85
40	MOTA	79	CB	SER	317	3.311		17.230	1.00	49.38
	MOTA	80	OG	SER	317	3.225	5.631 5.601	18.114	1.00	39.72
	MOTA	81	C	SER	317	5.696		18.407	1.00	40.21
	MOTA	82	0	SER	317	6.011	4.446 6.220	17.043	1.00	38.35
	MOTA	83	N	ALA	318	6.182	5.540	16.153	1.00	36.96
45	MOTA	84	CA	ALA	318	7.114	6.448	14.986		
	ATOM	85	CB	ALA	318	7.485		16.920		
	MOTA	86	С	ALA	318	8.375	5.137	16.844		
	MOTA	87	0	ALA	318	8.820	3.992	17.664		
	MOTA	88	N	LEU	319	8.938	6.089			
50	MOTA	89	CA	LEU	319	10.161	5.854	18.438		
	ATOM	90	CB	LEU	319	10.660	7.174	19.040		
	MOTA	91	CG	LEU	319	11.136		18.071		
	MOTA	92	CD1	LEU	319	11.714		18.857		
	MOTA	93	CD2	LEU	319	12.182		17.140		
55	MOTA	94	С	LEU		9.965		19.549		
	ATOM	95	0	LEU		10.779				
	MOTA	96	N	LEU		8.879				_
	ATOM	97	CA	LEU		8.567				
	MOTA	98	CB	LEU		7.239				
60	MOTA	99	CG	LEU		7.236				
	MOTA	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96

5	MOTA	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
	ATOM	102	С	LEU	320	8.466	2.642	20.843	1.00	41.11
	ATOM	103	0	LEU	320	8.971	1.697	21.443	1.00	41.87
	ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
	MOTA	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
10	ATOM	106	CB	ASP	321	6.669	1.372	17.860	1.00	48.39
	ATOM	107	CG	ASP	321	5.206	1.318	18.255	1.00	52.39
	ATOM	108	OD1	ASP	321	4.901	1.422	19.464	1.00	53.56
	MOTA	109	OD2	ASP	321	4.357	1.172	17.346	1.00	55.81
	ATOM	110	С	ASP	321	8.911	0.565	18.568	1.00	44.37
15	ATOM	111	0	ASP	321	9.030	-0.661	18.533	1.00	44.67
	ATOM	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	ATOM	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
	ATOM	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
	ATOM	115	C	ALA	322	12.148	0.513	18.769	1.00	35.52
20	ATOM	116	0	ALA	322	13.219	-0.020	18.473	1.00	36.11
	ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	ATOM	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
	ATOM	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
	ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
25	ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
	ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
	ATOM	124	C	GLU	323	13.205	-0.978	21.110	1.00	38.02
	ATOM	125	Ö	GLU	323	12.425	-1.931	20.999	1.00	38.37
30	ATOM	126	N	PRO	324	14.527	-1.151	21.225	1.00	36.03
	ATOM	127	CD	PRO	324	15.522	-0.069	21.225	1.00	36.69
	ATOM	128	CA	PRO	324	15.158	-2.474	21.240	1.00	36.42
	ATOM	129	CB	PRO	324	16.633	-2.166	21.003	1.00	35.75
	ATOM	130	CG	PRO	324	16.811	-0.807	21.610	1.00	35.46
35	ATOM	131	C	PRO	324	14.940	-3.162	22.583	1.00	35.75
-	ATOM	132	Ö	PRO	324	14.616	-2.517	23.580	1.00	34.97
	ATOM	133	N	PRO	325	15.134	-4.485	22.631	1.00	35.24
	ATOM	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
	ATOM	135	CA	PRO	325	14.942	-5.208	23.889	1.00	34.65
40	ATOM	136	CB	PRO	325	14.753	-6.652	23.439	1.00	35.83
	ATOM	137	CG	PRO	325	15.589	-6.743	22.200	1.00	34.88
	ATOM	138	c	PRO	325	16.132	-5.070	24.824	1.00	34.51
	MOTA	139	ō	PRO	325	17.237	-4.723	24.399	1.00	29.92
	ATOM	140	N	ILE	326	15.899	-5.322	26.106	1.00	33.62
45	ATOM	141	CA	ILE	326	16.975	-5.265	27.075	1.00	35.02
	ATOM	142	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
	ATOM	143	CG2	ILE	326	17.557	-5.110	29.504	1.00	38.70
	ATOM	144	CG1	ILE	326	15.987	-3.431	28.466	1.00	40.48
	ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
50	ATOM	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
	ATOM	147	Õ	ILE	326	16.875	-7.634	27.103	1.00	34.88
	ATOM	148	N	LEU	327	18.840	-6.784	26.745	1.00	29.64
	ATOM	149	CA	LEU	327	19.493	-8.083	26.743	1.00	29.54
	ATOM	150	CB	LEU	327	20.528	-8.135	25.587	1.00	
55	ATOM	151	CG	LEU	327	19.978	-7.800	23.387	1.00	27.76 29.02
	ATOM	152	CD1	LEU	327	21.068				
	ATOM	153	CD2	LEU	327	18.775	-7.993 -8.688	23.139 23.891	1.00	28.76
	ATOM	154	C	LEU	327	20.156	-8.438			31.26
	ATOM	155	0	LEU	327	20.156	-8.438 -7.578	28.030	1.00	31.21
60	ATOM	156	N	TYR	328	20.393	-7.578 -9.725	28.891	1.00	30.12
	ATOM	157	CA	TYR	328	21.087		28.181	1.00	30.99
			~	111	340	21.00/	-10.223	29.381	1.00	30.95

5	ATOM	158	СВ	TYR	328	20.409	-11.520	29.842	1.00	33.38
•	ATOM	159	CG	TYR	328	19.194	-11.272	30.686	1.00	33.05
	MOTA	160	CD1	TYR	328	19.253	-11.398	32.071	1.00	31.92
			CE1		328	18.152	-11.114	32.864	1.00	36.01
	MOTA	161		TYR		17.996	-10.862	30.110	1.00	36.05
10	MOTA	162	CD2	TYR	328			30.899	1.00	37.27
10	ATOM	163	CE2	TYR	328	16.880	-10.574			37.66
	ATOM	164	CZ	TYR	328	16.973	-10.702	32.274	1.00	
	MOTA	165	OH	TYR	328	15.896	-10.397	33.071	1.00	44.66
	MOTA	166	С	TYR	328	22.529	-10.520	29.067	1.00	33.66
	MOTA	167	0	TYR	328	22.884	-10.744	27.910	1.00	34.78
15	ATOM	168	N	SER	329	23.359	-10.496	30.103	1.00	33.97
	ATOM	169	CA	SER	329	24.767	-10.800	29.962	1.00	37.29
	ATOM	170	CB	SER	329	25.526	-10.342	31.204	1.00	36.51
	ATOM	171	OG	SER	329	26.787	-10.965	31.282	1.00	37.13
	ATOM	172	С	SER	329	24.835	-12.317	29.832	1.00	40.43
20	ATOM	173	0	SER	329	23.980	-13.028	30.363	1.00	40.11
	ATOM	174	N	GLU	330	25.845	-12.811	29.128	1.00	41.40
	ATOM	175	CA	GLU	330	25.992	-14.242	28.928	1.00	47.43
	MOTA	176	CB	GLU	330	26.423	-14.524	27.484	1.00	48.64
						25.278	-14.870	26.542	1.00	50.20
25	MOTA	177	CG	GLU	330		-15.405	25.198	1.00	53.25
25	ATOM	178	CD	GLU	330	25.765				53.27
	ATOM	179	OE1	GLU	330	25.909	-16.640	25.062	1.00	
	MOTA	180	OE2	GLU	330	26.004	-14.590	24.280	1.00	51.80
	MOTA	181	C	GLU	330	26.999	-14.852	29.893	1.00	49.67
	MOTA	182	0	GLU	330	28.207	-14.741	29.696	1.00	50.11
30	ATOM	183	N	TYR	331	26.498	-15.493	30.942	1.00	53.62
	MOTA	184	CA	TYR	331	27.373	-16.130	31.921	1.00	58.16
	ATOM	185	CB	TYR	331	28.092	-15.078	32.774	1.00	59.55
	MOTA	186	CG	TYR	331	27.239	-14.460	33.860	1.00	63.08
	MOTA	187	CD1	TYR	331	26.656	-13.205	33.682	1.00	64.50
35	ATOM	188	CE1	TYR	331	25.864	-12.630	34.676	1.00	65.99
	ATOM	189	CD2	TYR	331	27.010	-15.128	35.065	1.00	63.52
	MOTA	190	CE2	TYR	331	26.219	-14.563	36.066	1.00	65.60
	ATOM	191	cz	TYR	331	25.648	-13.314	35.864	1.00	67.20
	MOTA	192	OH	TYR	331	24.855	-12.753	36.839	1.00	67.40
40	ATOM	193	С	TYR	331	26.603	-17.080	32.823	1.00	59.05
	ATOM	194	Ō	TYR	331	25.393	-16.942	33.002	1.00	59.22
	ATOM	195	N	ASP	332	27.320	-18.045	33.387	1.00	61.62
	ATOM	196	CA	ASP	332		-19.026	34.281	1.00	64.20
	ATOM	197	CB	ASP	332		-20.194	34.500	1.00	65.99
45	ATOM	198	CG	ASP	332		-21.516	34.648	1.00	68.11
75	ATOM	199	OD1	ASP	332		-22.564	34.351	1.00	69.54
	ATOM	200	OD2	ASP	332		-21.505	35.060	1.00	67.40
			C C				-18.371	35.619	1.00	63.33
	ATOM	201		ASP	332			36.406	1.00	63.90
60	MOTA	202	0	ASP	332		-18.073			
50	ATOM	203	N	PRO	333		-18.148	35.896	1.00	
	ATOM	204	CD	PRO	333		-18.509	35.053	1.00	
	MOTA	205	CA	PRO	333		-17.521	37.154	1.00	
	MOTA	206	CB	PRO	333		-17.333	36.993	1.00	
	MOTA	207	CG	PRO	333		-17.611	35.556	1.00	
55	MOTA	208	C	PRO	333		-18.419	38.332	1.00	
	MOTA	209	0	PRO	333	25.129	-17.964	39.468	1.00	63.28
	ATOM	210	N	THR	334	25.160	-19.704	38.037	1.00	64.26
	ATOM	211	CA	THR	334	25.475	-20.697	39.050	1.00	66.09
	ATOM	212	CB	THR	334		-22.080	38.645	1.00	66.90
60	ATOM	213	OG1	THR	334		-22.513	37.439	1.00	68.06
	ATOM	214	CG2	THR	334		-22.012	38.411	1.00	67.57
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5	ATOM	215	С	THR	334	26.982	-20.804	39.269	1.00	65.67
	ATOM	216	0	THR	334	27.432	-21.323	40.289	1.00	64.77
	MOTA	217	N	ARG	335	27.759	-20.308	38.313	1.00	65.65
	ATOM	218	CA	ARG	335	29.214	-20.360	38.421	1.00	66.60
	ATOM	219	CB	ARG	335	29.835	-20.500	37.030	1.00	66.74
10	MOTA	220	С	ARG	335	29.757	-19.113	39.123	1.00	67.09
	ATOM	221	0	ARG	335	29.100	-18.071	39.148	1.00	67.31
	ATOM	222	N	PRO	336	30.968	-19.207	39.702	1.00	67.62
	ATOM	223	CD	PRO	336	31.820	-20.408	39.713	1.00	67.30
	ATOM	224	CA	PRO	336	31.601	-18.086	40.410	1.00	67.42
15	ATOM	225	CB	PRO	336	32.982	-18.621	40.783	1.00	66.43
	ATOM	226	CG	PRO	336	32.829	-20.097	40.779	1.00	67.52
	ATOM	227	С	PRO	336	31.701	-16.828	39.561	1.00	68.26
	ATOM	228	0	PRO	336	31.996	-16.895	38.371	1.00	69.04
	MOTA	229	N	PHE	337	31.460	-15.681	40.183	1.00	69.49
20	MOTA	230	CA	PHE	337	31.529	-14.408	39.480	1.00	71.39
	MOTA	. 231	CB	PHE	337	30.818	-13.323	40.294	1.00	72.31
	ATOM	232	CG	PHE	337	31.219	-11.924	39.921	1.00	73.21
	ATOM	233	CD1	PHE	337	30.632	-11.287	38.833	1.00	72.82
	ATOM	234	CD2	PHE	337	32.191	-11.245	40.653	1.00	73.43
25	ATOM	235	CEl	PHE	337	31.006	-9.993	38.479	1.00	73.28
	ATOM	236	CE2	PHE	337	32.573	-9.950	40.306	1.00	73.00
	ATOM	237	CZ	PHE	337	31.980	-9.323	39.217	1.00	72.90
	ATOM	238	С	PHE	337	32.985	-14.013	39.245	1.00	71.38
	ATOM	239	0	PHE	337	33.336	-13.487	38.189	1.00	71.56
30	ATOM	240	N	SER	338	33.825	-14.273	40.241	1.00	71.53
	ATOM	241	CA	SER	338	35.248	-13.947	40.172	1.00	70.98
	ATOM	242	CB	SER	338	35.957	-14.487	41.414	1.00	70.43
	ATOM	243	OG	SER	338	35.547	-15.818	41.679	1.00	69.59
	ATOM	244	С	SER	338	35.931	-14.504	38.924	1.00	71.20
35	ATOM	245	0	SER	338	36.951	-13.972	38.475	1.00	71.35
	MOTA	246	N	GLU	339	35.368	-15.573	38.369	1.00	70.20
	MOTA	247	CA	GLU	339	35.930	-16.215	37.183	1.00	69.48
	MOTA	248	CB	GLU	339	35.279	-17.585	36.971	1.00	71.07
	ATOM	249	CG	GLU	339	35.996	-18.740	37.656	1.00	72.60
40	MOTA	250	CD	GLU	339	35.382	-20.089	37.318	1.00	74.26
	MOTA	251	OE1	GLU	339	34.786	-20.220	36.227	1.00	73.51
	ATOM	252	OE2	GLU	339	35.496	-21.020	38.144	1.00	76.44
	MOTA	253	C	GLU	339	35.770	-15.385	35.910	1.00	68.15
	ATOM	254	0	GLU	339		-15.216	35.144	1.00	68.99
45	ATOM	255	N	ALA	340	34.562	-14.874	35.694	1.00	64.41
	ATOM	256	CA	ALA	340	34.246	-14.083	34.507	1.00	60.69
	ATOM	257	CB	ALA	340	32.767	-13.709	34.523	1.00	61.17
	ATOM	258	С	ALA	340	35.096	-12.824	34.326	1.00	57.00
	ATOM	259	0	ALA	340	35.634	-12.270	35.287	1.00	57.46
50	ATOM	260	N	SER	341	35.215	-12.388	33.076	1.00	52.15
	ATOM	261	CA	SER	341	35.972	-11.188	32.736	1.00	46.53
	ATOM	262	CB	SER	341	36.839	-11.439	31.497	1.00	48.64
	ATOM	263	OG	SER	341	37.184	-10.226	30.846	1.00	46.48
	ATOM	264	C	SER	341	34.957		32.444	1.00	43.52
55	ATOM	265	0	SER	341	34.090	-10.248	31.589	1.00	39.92
	ATOM	266	N	MET	342	35.052	-8.978	33.166	1.00	41.24
	MOTA	267	CA	MET	342	34.121	-7.875	32.960	1.00	42.46
	MOTA	268	CB	MET	342	34.449	-6.723	33.912	1.00	45.61
	MOTA	269	CG	MET	342	33.228	-6.089	34.560	1.00	52.39
60	ATOM	270	SD	MET	342	31.791	-7.201	34.631	1.00	57.92
	MOTA	271	CE	MET	342	31.999	-7.881	36.239	1.00	56.18

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5	ATOM	272	С	MET	342	34.124	-7.365	31.516	1.00	
	MOTA	273	0	MET	342	33.063	-7.121	30.938	1.00	39.23
	MOTA	274	N	MET	343	35.307	-7.204	30.930	1.00	38.72
	ATOM	275	CA	MET	343	35.395	-6.708	29.558	1.00	38.50
	ATOM	276	CB	MET	343	36.838	-6.318	29.216	1.00	41.15
10	ATOM	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	ATOM	278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
	ATOM	279	CE	MET	343	36.113	-3.358	28.987	1.00	40.45
	ATOM	280	C	MET	343	34.880	-7.741	28.561	1.00	35.36
	ATOM	281	Ö	MET	343	34.368	-7.384	27.501	1.00	35.51
15	ATOM	282	N	GLY	344	35.017	-9.020	28.902	1.00	35.53
13			CA	GLY	344	34.533	-10.072	28.024	1.00	33.41
	ATOM	283					-10.063	28.047	1.00	31.74
	ATOM	284	C	GLY	344	33.015		27.019	1.00	29.58
	ATOM	285	0	GLY	344	32.359	-10.233			
	ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
20	MOTA	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	MOTA	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
	MOTA	289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
	ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
	ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
25	ATOM	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
	ATOM	293	0	LEU	345	29.479	-8.757	27.868	1.00	30.29
	ATOM	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
	ATOM	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
	ATOM	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
30	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
20	ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
	ATOM	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
	MOTA	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
	ATOM	301	0	LEU	346	29.869	-5.765	25.955	1.00	29.13
35	ATOM	302	Ŋ	THR	347	31.839	-6.816	26.212	1.00	30.47
33			CA	THR	347	32.086	-6.911	24.781	1.00	30.93
	MOTA	303		THR	347	32.000	-7.501	24.497	1.00	29.97
	ATOM	304	CB				-6.604	24.982	1.00	35.40
	MOTA	305	OG1	THR	347	34.481		23.004	1.00	33.58
40	ATOM	306	CG2	THR	347	33.666	-7.707	24.122	1.00	31.97
40	MOTA	307	C	THR	347	31.036	-7.804			30.75
	ATOM	308	0	THR	347	30.516	-7.486	23.049	1.00	29.31
	MOTA	309	N	ASN	348	30.737	-8.926	24.768	1.00	
	MOTA	310	CA	ASN	348	29.757		24.242	1.00	32.63
	ATOM	311	CB	ASN	348		-11.161	25.065	1.00	31.64
45	ATOM	312	CG	ASN	348		-12.117	24.662	1.00	39.14
	MOTA	313	OD1	ASN	348		-12.078	25.220	1.00	41.91
	ATOM	314	ND2	ASN	348	28.920		23.683	1.00	42.05
	MOTA	315	С	ASN	348	28.361		24.262	1.00	29.02
	ATOM	316	0	ASN	348	27.558	-9.477	23.353	1.00	32.76
50	ATOM	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
	MOTA	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58
	MOTA	319	CB	LEU	349	26.650	-7.148	26.795	1.00	26.56
	ATOM	320	CG	LEU	349	25.376		27.050	1.00	33.67
	ATOM	321	CD1	LEU	349	24.140		26.840	1.00	28.82
55	ATOM	322	CD2	LEU	349	25.392		28.471	1.00	33.11
20	ATOM	323	C	LEU	349	26.638		24.319	1.00	28.07
	ATOM	324	0	LEU	349	25.616		23.629	1.00	25.22
	ATOM	325	N	ALA	350	27.675		24.157	1.00	28.50
			CA			27.668		23.148		28.46
60	ATOM	326		ALA	350			23.148		
60	ATOM	327	CB	ALA	350	28.972				28.75
	MOTA	328	С	ALA	350	27.468	-5.461	21.750	1.00	20./3

5	MOTA	329	0	ALA	350	26.649	-4.958	20.983	1.00	30.90
	ATOM	330	N	ASP	351	28.213	-6.509			
	ATOM	331	CA	ASP	351	28.093	-7.143			
	ATOM	332	CB	ASP	351	29.036	-8.345			
	ATOM	333	CG	ASP	351	30.498	-7.940		_	
10	ATOM	334	OD1	ASP	351	31.354	-8.831			
	MOTA	335	OD2	ASP	351	30.789	-6.738	19.784		
	ATOM	336	С	ASP	351	26.661	-7.600	19.813		
	ATOM	337	0	ASP	351	26.193	-7.458			
	ATOM	338	N	ARG	352	25.968	-8.150	18.687		
15	ATOM	339	CA	ARG	352	24.593		20.811		
	ATOM	340	CB	ARG	352	24.148	-8.602	20.605		
	ATOM	341	CG	ARG	352		-9.534	21.752		
	ATOM	342	CD	ARG	352	24.567		21.532	1.00	
	ATOM	343	NE	ARG		24.128	-11.911	22.666		
20	ATOM	344	CZ		352	24.898		23.879		
	ATOM	345	NH1	ARG	352	24.364		25.054		
	ATOM	346		ARG	352	23.050	-11.251	25.177	1.00	31.18
	ATOM	347	NH2 C	ARG	352	25.144	-11.148	26.104	1.00	32.03
	ATOM			ARG	352	23.642	-7.411	20.502	1.00	27.16
25	ATOM	348	0	ARG	352	22.702	-7.426	19.708	1.00	26.65
23	ATOM	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
		350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
	ATOM	351	CB	GĽŨ	353	23.461	-4.204	22.365	1.00	24.91
	ATOM	352	CG	GĻU	353	23.147	-4.669	23.771	1.00	27.93
30	ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
30	ATOM	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
	ATOM	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
	ATOM	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
	ATOM	357	0	GLŲ	353	22.169	-3.826	19.467	1.00	28.71
25	ATOM	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
35	ATOM	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
	ATOM	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
	ATOM	361	CG	LEU	354	26.372	-3.257	16.351	1.00	29.24
	ATOM	362	CD1	LEU	354	26.243	-1.774	16.722	1.00	26.59
40	MOTA	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
40	ATOM	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
	ATOM	365	0	LEU	354	23.074	-3.475	16.152	1.00	24.00
	ATOM	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
•	ATOM	367	CA	٧AŢ٠	355	22.386	-6.125	15.844	1.00	
	ATOM	368	CB	VAL	355	22.259	-7.655	15.975	1.00	29.45
45	ATOM	369	CG1	VAL	355	21.423	-8.205	14.834		31.76
	ATOM	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	33.55
	ATOM	371	С	VAL	355	21.020	-5.499		1.00	31.36
	ATOM	372	0	VAL	355	20.382	-5.039	16.035	1.00	27.71
	ATOM	373	N	HIS	356	20.580		15.080	1.00	29.61
50	ATOM	374	CA	HIS	356	19.291	-5.473	17.288	1.00	27.76
	ATOM	375	CB	HIS	356		-4.906	17.627	1.00	28.35
	ATOM	376	CG	HIS	356	18.936	-5.231	19.079	1.00	31.12
	ATOM	377	CD2	HIS		18.602	-6.675	19.307	1.00	35.93
	ATOM	378	ND1	HIS	356	19.352	-7.700°	19.779	1.00	33.95
55	ATOM	379	CE1		356	17.363	-7.208	19.018	1.00	36.62
	ATOM	380		HIS	356	17.364	-8.499	19.304	1.00	33.33
	ATOM	381	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
	ATOM		C	HIS	356	19.300	-3.398	17.412	1.00	28.25
		382	0	HIS	356	18.272	-2.812	17.100	1.00	28.99
60	ATOM	383	N	MET	357	20.457	-2.765	17.574	1.00	25.31
UU	ATOM	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	ATOM	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61

						00 011	0.736	17.699	1.00	24.66
5	ATOM	386	CG	MET	357	22.011	0.736	17.859	1.00	27.30
	MOTA	387	SD	MET	357	23.732	1.290	19.514	1.00	23.62
	ATOM	388	CE	MET	357	24.140	0.672		1.00	24.83
	MOTA	389	C	MET	357	20.256	-1.011	15.898	1.00	26.78
	MOTA	390	0	MET	357	19.619	-0.003	15.569		26.25
10	ATOM	391	N	ILE	358	20.757	-1.874	15.020	1.00	30.33
	ATOM	392	CA	ILE	358	20.553	-1.721	13.576	1.00	
	MOTA	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.86
	ATOM	394	CG2	ILE	358	20.759	-2.860	11.334	1.00	33.68
	ATOM	395	CG1	ILE	358	22.728	-2.799	12.874	1.00	36.89
15	MOTA	396	CD1	ILE	358	23.299	-1.469	12.451	1.00	39.10
	ATOM	397	С	ILE	358	19.055	-1.721	13.310	1.00	32.20
	MOTA	398	0	ILE	358	18.519	-0.817	12.662	1.00	32.02
	ATOM	399	N	ASN	359	18.379	-2.748	13.814	1.00	33.12
	ATOM	400	CA	ASN	359	16.945	-2.861	13.638	1.00	33.35
20	ATOM	401	CB	ASN	359	16.434	-4.101	14.363	1.00	37.59
	ATOM	402	CG	ASN	359	16.739	-5.374	13.627	1.00	44.38
	ATOM	403	OD1	ASN	359	17.045	-5.329	12.437	1.00	47.35
	MOTA	404	ND2	ASN	359	16.673 [.]	-6.508	14.320	1.00	42.48
	ATOM	405	C	ASN	359	16.224	-1.634	14.149	1.00	32.74
25	ATOM	406	O	ASN	359	15.261	-1.163	13.530	1.00	31.39
	ATOM	407	N	TRP	360	16.706	-1.104	15.264	1.00	27.92
	ATOM	408	CA	TRP	360	16.102	0.087	15.842	1.00	29.47
	ATOM	409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
	ATOM	410	CG	TRP	360	16.522	1.747	17.707	1.00	30.40
30	ATOM	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
30	ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
	MOTA	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
	ATOM	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
35	ATOM	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
55	ATOM	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
	ATOM	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
	ATOM	419	C	TRP	360	16.312	1.296	14.926	1.00	27.90
	ATOM	420	0	TRP	360	15.360	2.002	14.581	1.00	28.83
40	ATOM	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
	ATOM	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
	ATOM	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
	ATOM	424	C	АLА	361	17.006	2.685	12.403	1.00	31.08
	ATOM	425	Ō	ALA	361	16.531	3.746	12.011	1.00	
45	ATOM	426	N	LYS	362	16.795	1.526	11.783	1.00	
	ATOM	427	CA	LYS	362	15.981	1.443	10.581		
	ATOM	428	CB	LYS	362	16.012	0.016	10.023		
	ATOM	429	CG	LYS	362	17.252	-0.281	9.198	1.00	
	ATOM	430	CD	LYS	362	17.547	-1.774	9.136	1.00	
50	ATOM	431	CE	LYS	362	18.852	-2.046	8.389	1.00	
30	ATOM	432	NZ	LYS	362	19.178	-3.507	8.288		
	ATOM	433	C	LYS	362	14.545	1.872	10.815	1.00	
	ATOM	434	Ö	LYS	362	13.821	2.168	9.859	1.00	37.95
	MOTA	435	N	ARG	363	14.134	1.921		1.00	34.23
55	ATOM	436	CA	ARG	363	12.770			1.00	36.04
כנ	ATOM	437		ARG	363	12.178	1.307			36.71
	ATOM	438		ARG	363	12.169				
		438		ARG	363	11.468				
	ATOM ATOM	440		ARG	363	10.161				
60		441		ARG		9.314				
OU	ATOM	442				9.642				
	ATOM	444	MUT	ANG	203	2.042				

5	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
	ATOM	444	С	ARG	363	12.654	3.743	12.943	1.00	37.40
	ATOM	445	0	ARG	363	11.567	4.199	13.303	1.00	38.22
	ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
	ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
10	ATOM	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
	MOTA	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
	MOTA	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30
	ATOM	451	С	VAL	364	13.360	6.591	12.171	1.00	33.19
	MOTA	452	0	VAL	364	14.028	6.531	11.146	1.00	33.04
15	ATOM	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
	ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
	ATOM	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
	ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
20	ATOM	458	C	PRO	365	12.756	8.878	10.321	1.00	37.19
	ATOM	459	Ō	PRO	365	13.430	9.726	10.907	1.00	40.29
	ATOM	460	N	GLY	366	12.878	8.624	9.023	1.00	34.78
	ATOM	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
	ATOM	462	C	GLY	366	15.168	8.722	8.007	1.00	34.26
25	ATOM	463	Ō	GLY	366	15.858	9.035	7.034	1.00	37.15
	ATOM	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
	ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	ATOM	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
	ATOM	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60
30	ATOM	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
	ATOM	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
	ATOM	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
	ATOM	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
35	ATOM	473	C	PHE	367	17.033	6.333	7.524	1.00	31.46
	ATOM	474	0	PHE	367	18.073	6.405	6.883	1.00	32.30
	ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
	MOTA	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
	ATOM	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
40	MOTA	478	CG1	VAL	368	15.543	2.447	6.843	1.00	41.48
	ATOM	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
	MOTA	480	С	VAL	368	15.965	5.523	4.673	1.00	40.06
	ATOM	481	0	VAL	368	16.156	4.992	3.579	1.00	41.66
	ATOM	482	N	ASP	369	15.608	6.798	4.798	1.00	38.65
45	ATOM	483	CA	ASP	369	15.465	7.646	3.621	1.00	37.15
	ATOM	484	CB	ASP	369	14.700	8.929	3.954	1.00	39.89
	ATOM	485	CG	ASP	369	13.254	8.671	4.302	1.00	45.59
	ATOM	486	OD1	ASP	369	12.686	7.672	3.806	1.00	46.34
	ATOM	487	OD2	ASP	369	12.681	9.472	5.074	1.00	49.13
50	MOTA	488	С	ASP	369	16.855	8.010	3.136	1.00	34.91
	MOTA	489	0	ASP	369	17.038	8.431	1.995	1.00	34.25
	MOTA	490	N	LEU	370	17.838	7.841	4.016	1.00	31.76
	MOTA	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
	MOTA	492	CB	LEU	370	20.020	8.339	5.003	1.00	28.81
55	ATOM	493	CG	ĻĒU	370	19.523	9.395	6.000	1.00	28.74
	MOTA	494	CD1	LEU	370	20.315	9.275	7.299	1.00	30.81
	ATOM	495	CD2	LEU	370	19.693	10.792	5.404	1.00	29.77
	ATOM	496	С	LEU	370	19.884	7.043	2.893	1.00	31.25
	ATOM	497	0	LEU	370	19.341	5.943	2.784	1.00	31.78
60	ATOM	498	N	TĤR	371	21.052	7.333	2.331	1.00	28.86
	ATOM	499	CA	THR	371	21.793	6.336	1.569	1.00	32.90

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5	» COM	500	CB	THR	371	22.979	6.944	0.818	1.00	33.44
2	ATOM	501	OG1	THR	371	23.880	7.523	1.766	1.00	34.59
	ATOM		CG2	THR	371	22.514	8.002	-0.178	1.00	32.63
	ATOM	502		THR	371	22.373	5.315	2.539	1.00	35.31
	ATOM	503	C	THR	371	22.536	5.591	3.733	1.00	31.27
10	ATOM	504	0		372	22.702	4.141	2.015	1.00	34.34
10	ATOM	505	N	LEU		23.273	3.073	2.822	1.00	35.46
	ATOM	506	CA	LEU	372		1.841	1.944	1.00	37.73
	ATOM	507	CB	LEU	372	23.518	0.704	2.515	1.00	42.43
	ATOM	508	CG	LEU	372	24.362		3.757	1.00	45.60
	ATOM	509	CD1	LEU	372	23.690	0.145		1.00	44.29
15	MOTA	510	CD2	LEU	372	24.534	-0.383	1.455	1.00	36.95
	MOTA	511	С	LEU	372	24.587	3.548	3.444		35.57
	MOTA	512	0	LEU	372	24.813	3.374	4.643	1.00	
	ATOM	513	N	HIS	373	25.442	4.159	2.627	1.00	35.68
	ATOM	514	CA	HIS	373	26.729	4.656	3.099	1.00	36.60
20	ATOM	515	CB	HIS	373	27.506	5.282	1.935	1.00	44.01
	ATOM	516	CG	HIS	373	28.538	6.280	2.360	1.00	50.69
	MOTA	517	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
	ATOM	518	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
	ATOM	519	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
25	ATOM	520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
	ATOM	521	С	HIS	373	26.575	5.669	4.244	1.00	36.22
	ATOM	522	0	HIS	373	27.350	5.650	5.201	1.00	33.05
	ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
	ATOM	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
30	ATOM	525	CB	ASP	374	24.354	8.603	4.713	1.00	30.12
50	MOTA	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
	ATOM	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
	ATOM	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
	ATOM	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
35	ATOM	530	0	ASP	374	25.152	7.275	7.587	1.00	27.04
33		531		GĻN	375	23.944	5.877	6.309	1.00	25.71
	MOTA	532	CA	GĻŅ	375	23.403	5.157	7.454	1.00	26.68
	ATOM		CB	GLN	375	22.424	4.077	6.993	1.00	29.70
	ATOM	533			375	21.101	4.616	6.484	1.00	29.16
40	ATOM	534	CG	GĽŅ GĽŅ	375 375	20.219	3.514	5.940	1.00	35.87
40	MOTA	535	CD			20.155	2.426	6.510	1.00	30.97
	ATOM	536	OE1	GLN	375	19.541	3.785	4.827	1.00	34.51
	ATOM	537	NE2	GLN	375		4.502	8.214	1.00	25.51
•	MOTA	538	C	GLN	375	24.556 24.585	4.513	9.442	1.00	28.14
	ATOM	539	0	GLN	375			7.475	1.00	26.62
45	ATOM	540	N	VAL	376	25.504	3.938	8.071	1.00	
	MOTA	541	CA	VAL	376	26.659	3.281	7.003	1.00	
	MOTA	542	CB	VAL	376	27.531	2.597	7.635	1.00	
	ATOM	543	CG1	VAL	376	28.812	2.071		1.00	
	MOTA	544	CG2	VAL	376	26.745	1.469	6.341		
50	ATOM	545	C	VAL	376	27.526	4.285	8.821	1.00	
	MOTA	546	0	VAL	376	27.953	4.029	9.948	1.00	
	MOTA	547	N	HIS	377	27.785	5.428	8.191		
	ATOM	548	CA	HIS	377	28.602	6.457	8.814		
	ATOM	549	CB	HIS	377	28.792	7.639	7.864		
55	ATOM	550	CG	HIS	377	29.508	8.791	8.488		
	ATOM	551	CD2	HIS	377	29.073	10.017	8.863		
	MOTA	552	ND1	HIS	377	30.846	8.740	8.823		
	MOTA	553	CE1	HIS	377	31.201	9.884	9.377		
	ATOM	554	NE2	HIS	377	30.144	10.677	9.413		
60	ATOM	555	C	HIS		27.983	6.954	10.114	1.00	
	ATOM	556	Ō	HIS		28.677	7.102	11.115	1.00	25.93

5	ATOM	557								
	ATOM	557 558		LEU		26.678	7.206		7 1.00	24.58
	ATOM	559		LEU		26.015	7.695			26.40
	ATOM	560		LEU		24.542	8.001		1.00	26.29
	ATOM	561		LEU	378	24.291	9.180		1.00	28.06
10	ATOM	562		LEU	378	22.778	9.353			27.66
	ATOM	563		LEU	378	24.911	10.458	10.642	1.00	30.08
	ATOM			LEU	378	26.120	6.695	12.459	1.00	28.55
	ATOM	564	0	LEU	378	26.379	7.075	13.605	1.00	24.76
	ATOM	565	N	LEU	379	25.919	5.414	12.153	1.00	24.29
15	ATOM	566	CA	LEU	379	26.000	4.388	13.182	1.00	27.03
13	ATOM	567	CB	LEU	379	25.401	3.073	12.667		28.53
	ATOM	568	CG	LEU	379	23.875	3.023	12.845	1.00	30.29
	ATOM	569	CD1	LEU	379	23.248	1.943	11.963		33.04
		570	CD2	LEU	379	23.563	2.759	14.312		29.45
20	ATOM	571	C	LEU	379	27.430	4.176	13.670		27.18
20	ATOM	572	0	LEU	379	27.653	3.979	14.866	1.00	25.95
	ATOM	573	N	GLU	380	28.402	4.236	12.762	1.00	25.86
	ATOM	574	CA	GĽŲ	380	29.786	4.054	13.173	1.00	27.58
	ATOM	575	CB	GĽÜ	380	30.730	4.036	11.968	1.00	30.36
25	ATOM	576	CG	GLU	380	32.172	3.785	12.380	1.00	37.98
23	ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	45.23
	ATOM	578	OE1	GLU	380	32.869	4.048	10.120	1.00	42.99
	ATOM	579	OE2	GLU	380	34.004	2.646	11.386	1.00	45.79
	ATOM	580	C	GLU	380	30.218	5.159	14.133	1.00	27.50
30	ATOM	581	0	GLU	380	31.056	4.937	15.010	1.00	26.67
30	ATOM	582	N	ACYS		29.637	6.339	13.965	0.75	24.89
	ATOM	583	N	BCYS		29.645	6.352	13.980	0.25	25.79
	ATOM	584	CA	ACYS		29.969	7.466	14.826	0.75	24.12
	ATOM	585	CA	BCYS		29.993	7.481	14.847	0.25	24.86
35	ATOM	586	CB	ACYS	381	29.621	8.781	14.122	0.75	25.96
33	ATOM	587	CB	BCYS	381	29.766	8.814	14.115	0.25	25.62
	ATOM	588	SG	ACYS	381	30.698	9.192	12.732	0.75	31.63
	ATOM	589	SG	BCYS	381	30.227	10.312	15.059	0.25	25.40
	ATOM	590	С	ACYS	381	29.237	7.422	16.162	0.75	22.07
40	ATOM	591	С	BCYS	381	29.211	7.498	16.159	0.25	23.97
40	ATOM	592	0	ACYS	381	29.812	7.730	17.206	0.75	21.97
	ATOM	593	0	BCYS	381	29.724	7.940	17.187	0.25	23.99
	ATOM	594	N	ALA	382	27.974	7.012	16.128	1.00	23.41
	ATOM	595	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
45	ATOM	596	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
43	ATOM	597	С	ALA	382	26.913	5.755	18.131	1.00	25.39
	ATOM	598	0	ALA	382	26.374	5.837	19.234	1.00	23.09
	ATOM	599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
	ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
50	ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
30	MOTA	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
	ATOM	603	CD2	TRP	383	29.797	1.347	18.803	1.00	27.31
	ATOM	604	CE2	TRP	383	31.182	1.484	18.579	1.00	28.24
	ATOM	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
55	ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	24.58
55	ATOM	607	NE1	TRP	383	31.342	2.239	17.446		24.58 27.35
	ATOM	608	CZ2	TRP	383	32.133	0.909	19.420		
	ATOM	609	CZ3	TRP	383	30.305	0.039	20.745		28.76
	ATOM	610	CH2	TRP	383	31.674	0.191	20.496		28.09
60	ATOM	611	C	TRP	383	27.356	3.309			29.77
60	ATOM	612	0	TRP	383	26.526				23.54
	ATOM	613	N	LEU	384	28.542	3.765			22.90
								~	1.00	20.37

_		c	C3	LEU	384	28.864	3.713	21.640	1.00	22.41
5	ATOM	614	CA	LEU	384	30.369	3.890	21.883	1.00	24.98
	ATOM	615	CB		384	30.824	3.645	23.336	1.00	27.33
	MOTA	616	CG	LEU		30.273	2.305	23.853	1.00	29.71
	ATOM	617	CD1	LEU	384	32.336	3.648	23.398	1.00	26.07
	ATOM	618	CD2	LEU	384	28.075	4.732	22.453	1.00	19.44
10	MOTA	619	C	LEU	384		4.458	23.595	1.00	23.24
	ATOM	620	0	LEU	384	27.706	5.909	21.885	1.00	20.80
	MOTA	621	И	GLU	385	27.807	6.895	22.612	1.00	21.32
	MOTA	622	CA	GLU	385	27.011		21.797	1.00	21.91
	ATOM	623	CB	GLU	385	26.861	8.177	21.705	1.00	21.61
15	ATOM	624	CG	GLU	385	28.115	9.020		1.00	29.53
	MOTA	625	CD	GLU	385	27.882	10.256	20.860		30.54
	ATOM	626	OE1	GLU	385	27.374	11.256	21.401	1.00	29.97
	ATOM	627	OE2	GLU	385	28.188	10.219	19.658	1.00	
	ATOM	628	С	GLU	385	25.616	6.292	22.836	1.00	22.26
20	ATOM	629	0	GLU	385	25.022	6.438	23.902	1.00	22.26
	MOTA	630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
	ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
	ATOM	632	CB	ILE	386	23.328	4.455	20.498	1.00	22.88
	ATOM	633	CG2	ILE	386	22.009	3.647	20.618	1.00	23.85
25	ATOM	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
-5	ATOM	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
	ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
	ATOM	637	Õ	ILE	386	22.823	3.818	23.746	1.00	24.75
	MOTA	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
30	ATOM	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
30	ATOM	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
		641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
	ATOM		CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
	ATOM	642		LEU	387	24.791	-0.631	22.652	1.00	26.29
25	ATOM	643	CD2	LEU	387	24.944	2.660	25.438	1.00	26.22
35	MOTA	644	С		387	24.287	2.204	26.386	1.00	23.55
	MOTA	645	0	LEU	388	25.751	3.713	25.554	1.00	23.92
	MOTA	646	N	MET		25.924	4.385	26.835	1.00	24.26
	ATOM	647	CA	MET	388	27.088	5.378	26.761	1.00	23.87
	ATOM	648	CB	MET	388		4.722	26.743	1.00	24.08
40	MOTA	649	CG	MET	388	28.440	5.992	26.736	1.00	27.70
	ATOM	650	SD	MET	388	29.726		27.078	1.00	21.74
	MOTA	651	CE	MET	388	31.139	5.041	27.321	1.00	23.33
	MOTA	652	С	MET	388	24.660	5.094	28.505		
	ATOM	653	0	MET	388	24.341	5.026	26.436		
45	ATOM	654		ILE	389	23.935	5.775			
	ATOM	655		ILE	389	22.729	6.440			
	MOTA	656		ILE	389	22.132	7.439		•	
	MOTA	657		ILE	389	21.413	6.705			
	MOTA	658	CG1	ILE	389	21.185	8.402			
50	ATOM	659	CD1	ILE	389	20.431	9.383			
	ATOM	660	С	ILE	389	21.694	5.401			
	ATOM	661	0	ILE	389	20.938	5.631			
	ATOM	662		GLY		21.679				
	ATOM	663		GLY		20.753	3.201			
55		664		GLY		21.133	2.719			
23	ATOM	665		GLY		20.275		29.348		
	ATOM	666		LEU		22.433	_			
	ATOM	667		LEU		22.955		_	1.00	
		668		LEU		24.476				28.37
40	ATOM	669		LEU		25.206				30.81
60										
	ATOM	670	, (1)1	, DEC			2.232			

5	ATOM	671	CD2	LEU	391	26.709	1.619	30.958	1.00	25.25
	ATOM	672	C	LEU	391	22.603	3.070	31.104	1.00	30.84
	ATOM	673	0	LEU	391	22.156	2.669	32.186	1.00	29.19
	ATOM	674	N	VAL	392	22.817	4.355	30.850	1.00	28.91
	ATOM	675	CA	VAL	392	22.506	5.369	31.851	1.00	28.86
10	ATOM	676	CB	VAL	392	22.923	6.770	31.353	1.00	30.08
10	ATOM	677	CG1	VAL	392	22.329	7.854	32.237	1.00	32.32
	ATOM	678	CG2	VAL	392		6.870		1.00	28.52
	ATOM	679	CG2	VAL	392	24.442 21.013	5.327	31.372 32.165	1.00	28.42
		680	0							30.38
15	ATOM ATOM	681	N	VAL	392	20.621	5.345	33.327	1.00	28.23
13		682		TRP	393	20.191	5.241	31.125	1.00	
	ATOM	682 683	CA	TRP	393	18.732	5.186	31.280	1.00	29.70
	ATOM		CB	TRP	393	18.066	5.046	29.906	1.00	30.09
	ATOM	684	CG	TRP	393	16.605	4.670	29.953	1.00	33.50
20	ATOM	685	CD2	TRP	393	15.516	5.499	30.369	1.00	31.76
20	MOTA	686	CE2	TRP	393	14.336	4.725	30.264	1.00	38.11
	ATOM	687	CE3	TRP	393	15.419	6.821	30.824	1.00	32.56
	ATOM	688	CD1	TRP	393	16.057	3.459	29.618	1.00	34.31
	ATOM	689	NE1	TRP	393	14.696	3.486	29.801	1.00	34.36
25	ATOM	690	CZ2	TRP	393	13.073	5.233	30.597	1.00	37.93
23	ATOM	691 602	CZ3	TRP	393	14.162	7.326	31.155	1.00	35.24
	ATOM	692	CH2	TRP	393	13.007	6.531	31.039	1.00	37.77
	ATOM	693 694	C	TRP	393	18.256	4.051	32.191	1.00	32.07
	ATOM	694	0	TRP	393	17.460	4.275	33.109	1.00	32.12
30	ATOM	695 696	N	ARG	394	18.738	2.837	31.957	1.00	31.90
30	ATOM	697	CA	ARG	394	18.288	1.729	32.787	1.00	36.63
	ATOM ATOM	698	CB CG	ARG	394	18.492	0.389	32.065	1.00	36.41
		699	CD	ARG	394	19.914	0.009	31.764	1.00	36.50
	MOTA			ARG	394	19.929	-1.132	30.748	1.00	36.34
35	MOTA	700	NE CZ	ARG	394	21.282	-1.561	30.417	1.00	33.97
33	ATOM ATOM	701 702		ARG	394	21.864	-1.350	29.239	1.00	31.61
		702	NH1	ARG	394	21.208	-0.715	28.281	1.00	32.42
	ATOM ATOM	703	NH2 C	ARG ARG	394 394	23.098 18.911	-1.784 1.697	29.022 34.180	1.00	29.81 36.69
	ATOM	705	0	ARG	394	18.445			1.00	37.07
40	ATOM	705	N	SER	395	19.954	0.966 2.492	35.048 34.395	1.00	33.63
40	ATOM	707	CA	SER	395	20.603	2.564	35.701		35.69
	ATOM	708	CB	SER	395	22.112	2.784	35.540	1.00	32.94
	ATOM	709	OG	SER	395	22.112	1.811	34.688	1.00	32.34
	ATOM	710	C	SER	395	20.010	3.713	36.531	1.00	36.44
45	ATOM	711	0	SER	395	20.389	3.713	37.687	1.00	38.68
	ATOM	712	N	MET	396	19.076	4.449	35.937	1.00	36.46
	ATOM	713	CA	MET	396	18.431	5.588	36.589	1.00	43.08
	ATOM	714	CB	MET	396	17.275	6.104	35.725	1.00	43.87
	ATOM	715	CG	MET	396	17.481	7.507	35.725	1.00	46.18
50	ATOM	716	SD	MET	396	15.962	8.278	34.581	1.00	49.58
50	ATOM	717	CE	MET	396	14.988	8.298		1.00	53.58
	ATOM	718	CE	MET	396	17.906	5.303	36.065 37.992	1.00	46.18
	ATOM	719	0	MET	396	18.125	6.089	38.913	1.00	46.18
	ATOM	720		GLU	397	17.215				
55	ATOM	721	N CA	GLU	397	16.645	4.180 3.821	38.152	1.00	49.39
55	ATOM	721	CB	GLU	397	15.296	3.821	39.444 39.246	1.00	52.12 55.34
	ATOM	723	CG	GLU	397	14.166	4.073	39.246	1.00	58.86
	ATOM	723	CD	GLU	397	13.195	3.448	37.891	1.00	63.28
	MOTA	725	OE1	GLU	397	13.195	2.925	36.854	1.00	64.68
60	ATOM	725 726	OE1	GLU	397	11.972	3.475	38.155	1.00	65.39
	ATOM	727	C	GLU	397	17.548	2.933	40.283	1.00	
	71011	161	_	بابدي	101	11.340	2.733	30.203	1.00	52.75

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£	3.TOM	700	_	GLU	397	17.071	2.187	41.139	1.00	53.96
5	ATOM	728	N	HIS	398	18.851	3.014	40.040	1.00	50.25
	ATOM	729		HIS	398	19.813	2.220	40.792	1.00	49.34
	ATOM	730	CA		398	20.271	1.018	39.963	1.00	52.04
	MOTA	731	CB	HIS		19.187	0.017	39.721	1.00	53.95
	MOTA	732	CG	HIS	398		-1.022	40.472	1.00	53.92
10	MOTA	733	CD2	HIS	398	18.750		38.608	1.00	55.91
	MOTA	734	ND1	HIS	398	18.374	0.054	38.685	1.00	55.53
	MOTA	735	CE1	HIS	398	17.482	-0.917	39.806	1.00	55.81
	ATOM	736	NE2	HIS	398	17.688	-1.585		1.00	47.44
	MOTA	737	C	HIS	398	20.999	3.084	41.196 40.730	1.00	44.91
15	ATOM	738	0	HIS	398	22.121	2.887	42.096	1.00	46.45
	MOTA	739	N	PRO	399	20.755	4.049		1.00	47.27
	MOTA	740	CD	PRO	399	19.443	4.300	42.721		45.35
	MOTA	741	CA	PRO	399	21.785	4.968	42.586	1.00	47.40
	ATOM	742	CB	PRO	399	21.127	5.631	43.793	1.00	
20	MOTA	743	CG	PRO	399	19.660	5.561	43.504	1.00	47.72
	ATOM	744	С	PRO	399	23.086	4.270	42.958	1.00	44.70
	ATOM	745	0	PRO	399	23.078	3.233	43.627	1.00	46.46 41.57
	MOTA	746	N	GLY	400	24.202	4.840	42.509	1.00	39.84
	ATOM	747	CA	GLY	400	25.506	4.281	42.813	1.00	
25	MOTA	748	C	GLY	400	25.907	3.047	42.022	1.00	37.85
	MOTA	749	0	GLY	400	27.027	2.560	42.176	1.00	40.48
	MOTA	750	N	LYS	401	25.012	2.537	41.180	1.00	36.39
	MOTA	751	CA	LYS	401	25.315	1.344	40.390	1.00	34.47
	MOTA	752	CB	LYS	401	24.562	0.130	40.947	1.00	36.12
30	MOTA	753	CG	LYS	401	24.633	-0.007	42.466	1.00	39.30 44.38
	MOTA	754	CD	LYS	401	24.288	-1.429	42.903	1.00	
	MOTA	755	CE	ГÂŻ	401	24.459	-1.605	44.408	1.00	46.68 53.37
	ATOM	756	NZ	LYS	401	24.968	-2.969	44.747	1.00	32.34
	MOTA	757	С	LYS	401	24.969	1.485	38.911	1.00	
35	MOTA	758	0	LYS	401	24.141	2.308	38.531	1.00	31.16
	MOTA	759	N	LEU	402	25.612	0.663	38.086	1.00	28.52
	MOTA	760	CA	LEU	402	25.358	0.658	36.648	1.00	29.06
	ATOM	761	CB	LEU	402	26.661	0.847	35.867	1.00	29.26
	MOTA	762	CG	ΓĔЙ	402	27.278	2.242	36.029	1.00	24.67
40	ATOM	763	CD1	ĻEU	402	28.623	2.310	35.310	1.00	27.47
	MOTA	764	CD2	LEU	402	26.312	3.277	35.482	1.00	24.93
	MOTA	765	C	LEU	402	24.755	-0.686	36.292	1.00	30.43
	MOTA	766	0	LEU	402	25.367	-1.727	36.535	1.00	31.36 31.07
	MOTA	767	N	LEU	403	23.552	-0.658	35.735	1.00	32.96
45	ATOM	768	CA	LEU	403	22.873	-1.880	35.335	1.00	
	MOTA	769	CB	ΓĒЙ	403	21.361	-1.693	35.434	1.00	33.86 39.29
	MOTA	770	CG	LEU	403	20.551	-2.991	35.415	1.00	
	ATOM	771	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
	MOTA	772	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
50	MOTA	773	С	LEU	403	23.255	-2.218	33.899	1.00	30.06
	MOTA	774	0	LEŲ	403	22.543	-1.870	32.956		31.63
	ATOM	775	N	PHE	404	24.383	-2.893	33.733		29.19
	MOTA	776	CA	PHE	404	24.834	-3.256	32.403		28.93
	MOTA	777	CB	PHE	404	26.201	-3.929	32.493		30.05
55	ATOM	778	CG	PHE	404	27.305	-2.998	32.926		30.78
	MOTA	779	CD1	PHE	404	27.794	-3.033	34.228		32.91
	MOTA	780	CD2	PHE	404	27.848	-2.078	32.030		
	MOTA	781	CEl	PHE	404	28.816	-2.160	34.638		
	MOTA	782	CE2	PHE	404	28.864	-1.205	32.423		
60	MOTA	783	CZ	PHE	404	29.350	-1.242	33.727		
	MOTA	784	С	PHE	404	23.809	-4.181	31.756	1.00	30.80

5	ATOM	785	0	PHE	404	23.625	-4.175	30.538	3 1.00	28.09
	ATOM	786	N	ALA	405	23.138	-4.967			
	ATOM	787	CA	ALA	405	22.104	-5.910			
	MOTA	788	CB	ALA	405	22.745	-7.172			
	ATOM	789	C	ALA	405	21.309	-6.237			
10	ATOM	790	0	ALA	405	21.785	-5.995			
	ATOM	791	N	PRO	406	20.088	-6.779			
	ATOM	792	CD	PRO	406	19.356	-7.102			
	ATOM	793	CA	PRO	406	19.303				
	ATOM	794	СВ	PRO	406	17.985	-7.101			
15	ATOM	795	CG	PRO	406	17.922	-7.654			
	ATOM	796	C	PRO	406	19.997	-7.153			_
	ATOM	797	Ö	PRO	406		-8.084			
	ATOM	798	N	ASN		19.698	-8.112	36.626		
	ATOM	799	CA		407	20.924	-8.877			
20	ATOM	800	CB	ASN	407	21.652	-9.847	35.712		38.85
	ATOM	801	CG	ASN	407	21.582	-11.243	35.083	1.00	39.69
	ATOM	802	OD1	ASN	407	22.232	-11.306	33.711	_	44.10
	ATOM	803		ASN	407	22.345	-10.296	33.009		37.78
	ATOM		ND2	ASN	407	22.660	-12.503	33.319	1.00	45.74
25	ATOM	804	C	ASN	407	23.100	-9.435	35.874	1.00	38.12
	ATOM	805	0	ASN	407	23.965	-10.256	36.178	1.00	39.81
	ATOM	806	N	LEU	408	23.364	-8.149	35.671	1.00	37.80
	ATOM	807	CA	LEU	408	24.713	-7.631	35.799	1.00	36.89
		808	CB	LEU	408	25.449	-7.720	34.459	1.00	36.09
30	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	35.08
30	ATOM	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	39.15
	ATOM	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	36.85
	ATOM	812	C	LEU	408	24.670	-6.187	36.286	1.00	40.55
	ATOM	813	0	LEU	408	24.646	-5.248	35.491	1.00	38.29
25	ATOM	814	N	LEU	409	24.644	-6.034	37.607	1.00	39.50
35	ATOM	815	CA	LEU	409	24.606	-4.733	38.257	1.00	41.00
	ATOM	816	CB	LEU	409	23.392	-4.658	39.184	1.00	43.69
	ATOM	817	CG	LEU	409	23.164	-3.382	39.993	1.00	47.35
	ATOM	818	CD1	LEU	409	22.848	-2.233	39.058	1.00	47.09
40	MOTA	819	CD2	LEU	409	22.014	-3.603	40.976	1.00	49.38
40	ATOM	820	C	LEU	409	25.894	-4.566	39.060	1.00	41.80
	MOTA	821	0	LEU	409	26.178	-5.358	39.960	1.00	
	ATOM	822	N	LEU	410	26.676	-3.544	38.727		41.00
	MOTA	823	CA	ΓĒΩ	410	27.931	-3.296	39.423	1.00 1.00	39.23
	ATOM	824	CB	LEU	410	29.106	-3.354	38.442		40.45
45	ATOM	825	CG	LEU	410	29.457	-4.660		1.00	41.59
	ATOM	826	CD1	LEU	410	30.972	-4.728	37.716	1.00	44.87
	ATOM	827	CD2	LEU	410	28.949	-5.872	37.554	1.00	45.41
	ATOM	828	С	LEU	410	27.946		38.484	1.00	47.02
	ATOM	829	Ō	LEU	410	27.361	-1.944	40.132	1.00	40.67
50	ATOM	830	N	ASP	411		-0.970	39.652	1.00	40.22
	ATOM	831	CA	ASP		28.610	-1.890	41.281	1.00	41.57
	ATOM	832	CB		411	28.717	-0.640	42.025	1.00	42.69
	ATOM	833	CG	ASP	411	28.490	-0.874	43.528	1.00	44.44
	ATOM	834		ASP	411	29.655	-1.578	44.210	1.00	46.70
55	ATOM		OD1	ASP	411	29.537	-1.849	45.426	1.00	51.44
		835	OD2	ASP	411	30.680	-1.861	43.553	1.00	48.79
	ATOM	836	C	ASP	411	30.088	-0.016	41.779	1.00	43.70
	ATOM	837	0	ASP	411	30.933	-0.610	41.107	1.00	38.48
	ATOM	838	N	ARG	412	30.295	1.181	42.321	1.00	46.78
60	ATOM	839	CA	ARG	412	31.554	1.905	42.171	1.00	49.97
60	ATOM	840	CB	ARG	412	31.601	3.090	43.138	1.00	51.28
	ATOM	841	CG	ARG	412	30.971	4.364	42.614	1.00	54.77
						- · -		012	1.00	Ja. / /

								42 216	1.00	54.61
5	ATOM	842	CD	ARG	412	31.644	5.580			56.53
	ATOM	843	NE	ARG	412	33.071	5.615			61.90
	ATOM	844	CZ	ARG	412	33.827	6.708	42.985		
	ATOM	845	NHl	ARG	412	33.291	7.866	43.356		63.48
	ATOM	846	NH2	ARG	412	35.120	6.645	42.682		61.21
10		847	C	ARG	412	32.771	1.026	42.429		50.29
10	MOTA	848	0	ARG	412	33.628	0.866	41.561	1.00	51.02
	ATOM		N	ASN	413	32.844	0.469	43.633	1.00	51.94
	ATOM	849		ASN	413	33.969	-0.375	44.021	1.00	53.15
	MOTA	850	CA		413	33.719	-0.980	45.403	1.00	55.88
	MOTA	851	CB	ASN		33.654	0.073	46.496	1.00	57.99
15	MOTA	852	CG	ASN	413	33.697	1.276	46.223	1.00	58.27
	ATOM	853	OD1	ASN	413		-0.375	47.742	1.00	57.90
	ATOM	854	ND2	ASN	413	33.551		43.013	1.00	53.95
	ATOM	355	C	ASN	413	34.235	-1.480	42.659	1.00	53.67
	ATOM	856	0	ASN	413	35.386	-1.743		1.00	55.33
20	MOTA	857	N	GLN	414	33.173	-2.129	42.547		55.42
	ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.44
	ATOM	859	CB	GLN	414	31.991	-3.904	41.343	1.00	
	ATOM	860	CG	GLN	414	31.645	-4.933	42.391	1.00	56.07
	ATOM	861	CD	ĠLN	414	30.203	-5.376	42.336	1.00	57.40
25	ATOM	862	OE1	GĻŅ	414	29.296	-4.536	42.402	1.00	60.22
23	ATOM	863	NE2	GLN	414	29.973	-6.664	42.199	1.00	57.27
		864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
	MOTA		0	GLN	414	34.654	-3.265	39.578	1.00	56.16
	ATOM	865		GLY	415	33.398	-1.430	39.910	1.00	57.07
	ATOM	866	N	GLY	415	33.849	-0.806	38.680	1.00	58.51
30	ATOM	867	CA		415	35.350	-0.582	38.689	1.00	61.10
	MOTA	868	C	GLY	415	36.023	-0.748	37.671	1.00	59.47
	ATOM	869	0	GLY		35.877	-0.211	39.851	1.00	62.77
	ATOM	870	N	LYS	416	37.305	0.041	40.011	1.00	65.49
	MOTA	871	CA	LYS	416		0.262	41.491	1.00	66.04
35	ATOM	872	CB	LYS	416	37.634		41.823	1.00	68.71
	ATOM	873	CG	LYS	416	38.121	1.663	42.613	1.00	70.98
	MOTA	874	CD	LYS	416	37.078	2.439	44.100	1.00	71.84
	ATOM	875	CE	ĻYS	416	37.404	2.448	44.100	1.00	71.95
	ATOM	876	NZ	ĻYS	416	36.225	2.079		1.00	66.41
40	MOTA	877	C	LYS	416	38.159	-1.105	39.472		67.15
	MOTA	878	0	LYS	416	39.361	-0.946	39.269	1.00	67.33
	MOTA	879	N	CYS	417	37.538	-2.257	39.238	1.00	68.16
	ATOM	880	CA	CYS	417	38.270	-3.414	38.741	1.00	
	ATOM	881	CB	CYS	417	37.951	÷4.642	39.602		70.88
45	ATOM	882		CYS	417	38.592	-4.549			
1.5	ATOM	883		CYS	417	38.015	-3.736			_
	ATOM	884		CYS	417	38.632	-4.653			
	ATOM	885		VAL		37.111	-2.994			
	ATOM	886		VAL		36.817	-3.226	35.218		
50		887		VAL		35.326	-2.917		1.00	
50						34.971	-1.503			59.13
	MOTA	888				35.072	-3.121			54.85
	MOTA	889				37.739	-2.362			58.37
	ATOM	890		VAL		37.739	-1.140			
	MOTA	891		VAL			-3.012			
55		892		GLU		38.463				
	MOTA	893		GLU		39.403	-2.328			
	ATOM	894		GLU		40.149				
	MOTA	895		GLU		39.385				
	MOTA	896	S CD	GLU		40.179				
60		897		GLU	J 419					_
٠,	ATOM	898		GLT.	J 419	40.546	-4.313	28.46	2 1.00	, 63.16

5	ATOM	899	С	OT 11	47.0	20 561		21 662	7 00	F2 05
5		900	0	GLU	419	38.761	-1.281	31.662	1.00	52.05
	ATOM			GLU	419	37.665	-1.481	31.131	1.00	49.82
	ATOM	901	N	GLY	420	39.465	-0.165	31.491	1.00	49.45
	ATOM	902 903	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
10	ATOM ATOM		C	GLY	420	37.895	1.767	31.254	1.00	44.55
10	ATOM	904 905	O N	GLY	420	37.417	2.705	30.619	1.00	42.08
	ATOM	905		MET	421	37.503	1.471	32.488	1.00	43.41
	ATOM	907	CA CB	MET	421	36.449	2.248	33.123	1.00	42.48
	ATOM	908	CG	MET	421	35.306	1.327	33.554	1.00	42.34
15	ATOM	909	SD	MET	421	34.590	0.635	32.396	1.00	38.22
13	ATOM	910	CE	MET MET	421 421	32.927	0.102	32.843	1.00	38.56
	ATOM	911	CE			32.003	1.699	32.766		35.54
	ATOM	912	0	MET MET	421 421	36.923	3.059	34.312	1.00	41.64
	ATOM	913	Ŋ	VAL	421	36.113 38.232	3.512 3.256	35.111	1.00	39.77
20	ATOM	914	CA	VAL	422	38.757	4.019	34.430 35.557	1.00	43.42 44.79
20	ATOM	915	CB	VAL	422	40.285	4.019	35.433	1.00	46.54
	ATOM	916	CG1	VAL	422	40.595	5.086	34.206	1.00	48.25
	ATOM	917	CG2	VAL	422	40.813	4.920	36.696	1.00	46.24
	ATOM	918	C	VAL	422	38.056	5.372	35.689	1.00	44.09
25	ATOM	919	0	VAL	422	37.691	5.783	36.783	1.00	44.12
	ATOM	920	N	GĻŲ	423	37.846	6.055	34.570	1.00	42.07
	ATOM	921	CA	GĽÚ	423	37.192	7.356	34.616	1.00	40.24
	ATOM	922	CB	GLU	423	37.909	8.338	33.684	1.00	44.02
	ATOM	923	CG	GLU	423	39.411	8.467	33.893	1.00	50.04
30	ATOM	924	CD	GLU	423	40.096	9.158	32.719	1.00	55.64
	MOTA	925	OE1	GLU	423	39.539	10.156	32.205	1.00	56.66
	MOTA	926	OE2	GĻŪ	423	41.188	8.703	32.306	1.00	58.02
	MOTA	927	С	GĻŲ	423	35.704	7.337	34.250	1.00	35.77
	MOTA	928	0	GĽÜ	423	34.881	7.955	34.919	1.00	33.20
35	MOTA	929	N	ΙĻĘ	ä24	35.345	6.617	33.197	1.00	36.16
	ATOM	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
	ATOM	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
	ATOM	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
40	ATOM	933	CG1	IĻĒ	424	34.204	4.617	31.296	1.00	34.46
4.0	ATOM	934	CD1	ΙĻĒ	424	33.857	3.955	29.978	1.00	34.67
	ATOM	935	C	ΙĻΕ	424	32.890	6.035	33.685	1.00	28.89
	ATOM	936	0	ΙĹΕ	424	31.729	6.443	33.632	1.00	26.49
	ATOM	937	N	PHE	425	33.261	5.091	34.542	1.00	29.26
45	ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	29.87
43	ATOM	939	CB	PHE	425	32.903	3.529	36.423	1.00	31.26
	ATOM	940	CG	PHE	425	31.948	2.496	36.959	1.00	32.17
	ATOM ATOM	941 942	CD1	PHE	425	31.124	2.783	38.048	1.00	33.70
	ATOM	943	CD2	PHE	425	31.881	1.230	36.381	1.00	30.64
50	ATOM	943	CE1 CE2	PHE	425	30.244	1.814	38.563	1.00	32.60
50	ATOM	945	CZ	PHE	425	31.010	0.256	36.881	1.00	31.55
	ATOM	946	C	PHE PHE	425	30.189	0.549	37.973	1.00	33.34
	ATOM	947	0	PHE	425 425	31.594	5.649	36.240	1.00	30.17
	ATOM	948	N	ASP	425	30.368	5.774	36.276	1.00	26.71
55	ATOM	949	CA	ASP	426	32.415	6.483	36.870	1.00	29.45
	ATOM	950	CB	ASP	426	31.893 33.031	7.587 8.291	37.661 38.401	1.00	32.29 33.49
	ATOM	951	CG	ASP	426	33.455	7.546	39.655	1.00	39.42
	ATOM	952	OD1	ASP	426	32.767	6.574	40.038	1.00	38.35
	ATOM	953	OD2	ASP	426	34.480	7.934	40.038	1.00	39.58
60	ATOM	954	C	ASP	426	31.133	8.592	36.806	1.00	29.02
	ATOM	955	Ō	ASP	426	30.154	9.175	37.257	1.00	31.34
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5	ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
,			CA	MET	427	30.919	9.736	34.675	1.00	28.63
	ATOM	957				31.744	9.912	33.407	1.00	26.83
	ATOM	958	CB	MET	427					
	MOTA	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
	MOTA	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
10	MOTA	961	CE		427	35.409	11.753	32.643	1.00	44.60
	ATOM	962	С	MET .	427	29.526	9.202	34.324	1.00	28.70
	ATOM	963	0	MET	427	28.536	9.947	34.302	1.00	25.01
	ATOM	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	ATOM	965	CA	LEU	428	28.173	7.292	33.730	1.00	27.60
15	ATOM	966	CB	LEU	428	28.379	5.824	33.332	1.00	28.00
	ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
	ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	ATOM	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	MOTA	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
20			0	LEU	428	26.041	7.743	34.743	1.00	27.07
20	ATOM	971					7.147	36.126	1.00	30.40
	MOTA	972	N	LEU	429	27.701		37.323	1.00	30.59
	ATOM	973	CA	LEU	429	26.859	7.251			
	MOTA	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
	MOTA	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
25	ATOM	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
	MOTA	977	CD2		429	26.825	4.573	38.903	1.00	34.66
	ATOM	978	C	LEU	429	26.319	8.681	37.466	1.00	30.46
	ATOM	979	0	ĻĒŪ	429	25.143	8.901	37.769	1.00	28.40
	ATOM	980	N	AĻ A	430	27.193	9.656	37.237	1.00	31.34
30	MOTA	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
	ATOM	982	CB	ALA	430	,28.017	11.951	37.078	1.00	31.29
	ATOM	983	С	ĄĻĄ	430	25.696	11.387	36.344	1.00	31.04
	ATOM	984	0	ALĄ	430	24.753	12.107	36.674	1.00	30.79
	ATOM	985	N	THR	431	25.802	10.854	35.128	1.00	30.30
35	ATOM	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
-	ATOM	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	ATOM	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
	ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
40	ATOM	991	0	THR	431	22.402	11.099	34.397	1.00	26.18
	ATOM	992	N	SER	432	23.520	9.253	35.037	1.00	28.11
	ATOM	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
	ATOM	994	CB	SER	432	22.639	7.177	36.008		
	ATOM	995	OG	SER	432	21.454	6.412	36.136	1.00	36.92
45	ATOM	996	C	SER	432	21.454	9.399	36.589	1.00	
43					432	20.433	9.576	36.613	1.00	
	ATOM	997	0	SER					0.75	
	ATOM	998	N	ASER		22.476	9.901	37.496		
	ATOM	999	N	BSER		22.474	9.906	37.500	0.25	31.10
50	ATOM	1000		ASER		22.002	10.715	38.605	0.75	35.68
50	MOTA	1001		BSER		21.985	10.717	38.608	0.25	32.21
	MOTA	1002		ASER		23.185	11.097	39.502	0.75	37.18
	ATOM	1003		BŞER		23.145	11.104	39.529	0.25	31.45
	ATOM	1004	OG	ASER		22.823	12.090	40.443	0.75	44.09
	ATOM	1005	OG	BSER		23.785	9.953	40.053	0.25	29.52
55	ATOM	1006	С	ASER	433	21.299	11.971	38.091	0.75	
	MOTA	1007		BSER		21.295	11.976	38.092	0.25	32.88
	ATOM	1008		ASER		20.257	12.373	38.612	0.75	35.34
	ATOM	1009		BSER		20.264	12.391	38.622	0.25	33.42
	ATOM	1010		ARG	434	21.867	12.579	37.054	1.00	
60	ATOM	1011		ARG	434	21.300	13.788	36.470	1.00	
- •	ATOM	1012		ARG	434	22.239	14.354	35.400	1.00	33.89
			-2							

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5	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
	ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
	MOTA	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
	ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
10	ATOM	1017	NH1 NH2	ARG	434	20.132	19.049	36.428	1.00	40.70
10	ATOM	1018		ARG	434	20.175	19.998	34.337	1.00	38.78
	ATOM	1019 1020	C 0	ARG	434 434	19.937	13.491 14.266	35.873 36.053	1.00	33.48 30.54
	MOTA MOTA	1020	N	ARG PHE	434	18.996 19.831	12.371	35.158	1.00	34.68
	ATOM	1021	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
15	ATOM	1022	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
13	ATOM	1023	CG	PHE	435	19.240	10.034	32.386	1.00	37.63
	ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
	ATOM	1025	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
	ATOM	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
20	ATOM	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
	ATOM	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
	ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49
	ATOM	1031	Ō	PHE	435	16.361	12.135	35.496	1.00	34.78
	ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
25	ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
	MOTA	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
	ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	ATOM	1036	CD	AŖG	436	17.648	8.459	40.810	1.00	48.09
	MOTA	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
30	MOTA	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
	ATOM	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
	MOTA	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	ATOM	1041	С	ARG	436	16.576	12.302	38.493	1.00	40.40
2.5	MOTA	1042	0	ARG	436	15.382	12.458	38.730	1.00	41.49
35	MOTA	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02
	ATOM	1044	CA	MĒT	437	17.090	14.546	39.245	1.00	41.02
	ATOM	1045	CB	MET	437	18.329	15.427	39.440	1.00	40.29
	MOTA	1046	C	MET	437	16.099	15.221	38.299	1.00	40.81
40	ATOM ATOM	1047 1048	O N	MET	437	15.111	15.805	38.734	1.00	42.46 39.02
40	ATOM	1048	CA	MET MET	438 438	16.367	15.127	37.001 35.988	1.00	40.11
	ATOM	1050	CB	MET	438	15.510 16.237	15.732 15.793	34.651	1.00	38.16
	MOTA	1051	CG	MET	438	17.352	16.794	34.601	1.00	41.52
·	ATOM	1052	SD	MET	438	17.999	16.862	32.943	1.00	43.94
45	ATOM	1053	CE	MET	438	16.698	17.748	32.096	1.00	39.96
	ATOM	1054	C	MEŢ	438	14.221	14.964	35.783	1.00	37.72
	ATOM	1055	Ö	MET	438	13.305	15.451	35.125	1.00	36.82
	ATOM	1056	N	ASN	439	14.155	13.759	36.337	1.00	38.81
	ATOM	1057	CA	ASN	439	12.981	12.919	36.174	1.00	40.77
50	ATOM	1058	CB	ASN	439	11.762	13.556	36.847	1.00	44.52
	ATOM	1059	CG	ASN	439	10.566	12.620	36.887	1.00	48.29
	ATOM	1060	OD1	ASN	439	10.721	11.400	36.964	1.00	48.48
	ATOM	1061	ND2	A:SN	439	9.365	13.189	36.829	1.00	50.23
	ATOM	1062	С	ASN	439	12.725	12.744	34.677	1.00	39.36
55	ATOM	1063	0	ASN	439	11.637	13.037	34.172	1.00	37.76
	ATOM	1064	N	ĻEU	440	13.749	12.274	33.972	1.00	37.65
	ATOM	1065	CA	ĻEU	440	13.655	12.052	32.532	1.00	35.22
	ATOM	1066	СВ	LEU	440	14.999	11.576	31.987	1.00	34.70
	ATOM	1067	CG	LEU	440	15.022	11.467	30.462	1.00	35.45
60	ATOM	1068	CD1	LEU	440	14.890	12.862	29.869	1.00	35.24
	ATOM	1069	CD2	LEU	440	16.297	10.795	29.999	1.00	35.30

5	ATOM	1070	C	LEU	440	12.587	11.024	32.196	1.00	36.48
	ATOM	1071	0	LEU	440	12.518	9.967	32.826	1.00	37.36
	ATOM	1072	N	GLN	441	11.763	11.328	31.197	1.00	36.82
	ATOM	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
	ATOM	1074	CB	GLN	441	9.431	11.211	30.443	1.00	38.23
10	ATOM	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	ATOM	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
	ATOM	1078	NE2	GLN	441	9.119	11.132	33.818	1.00	44.06
	ATOM	1079	С	GLN	441	11.099	9.565	29.585	1.00	38.48
15	ATOM	1080	0	GLN	441	11.923	9.976	28.763	1.00	35.80
	ATOM	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
	ATOM	1082	CA	GLY	442	10.792	7.468	28.401	1.00	37.72
	ATOM	1083	C	GLY	442	10.599	8.112	27.043	1.00	36.88
	ATOM	1084	Ö	GLY	442	11.381	7.877	26.123	1.00	33.72
20	ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	ATOM	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
	ATOM	1087	CB	GLU	443	7.956	10.379	25.764	1.00	
	ATOM	1088	CG	GĽŪ	443	6.723·	9.488	25.879	1.00	47.76
	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
25	ATOM	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
	ATOM	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13
	ATOM	1092	C	GLU	443.	10.408	10.551	25.311	1.00	35.27
	ATOM	1093	Ö	GLU	443	10.759	10.704	24.145	1.00	33.85
	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	32.09
30	ATOM	1095	CA	ĞLU	444	12.097	12.095	26.126	1.00	33.92
	ATOM	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
	ATOM	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
	ATOM	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	ATOM	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
35	ATOM	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
	ATOM	1101	C	GLU	444	13.356	11.305	25.770	1.00	33.59
	MOTA	1102	Ō	ĢĻŲ	444	14.085	11.670	24.842	1.00	33.35
	ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
	ATOM	1104	CA	PHE	445	14.753	9.357	26.276	1.00	32.49
40	ATOM	1105	CB	PHE	445	14.703	8.139	27.203	1.00	29.35
	ATOM	1106	CG	PHE	445	15.667	7.047	26.828	1.00	30.78
	ATOM	1107	CD1	PHE	445	17.036	7.201	27.030	1.00	28.25
	ATOM	1108	CD2	PHE	445	15.205	5.863	26.266	1.00	30.62
	ATOM	1109	CE1	PHE	445	17.933	6.195	26.675	1.00	28.67
45	ATOM	1110	CE2	PHE	445	16.095	4.848	25.908	1.00	31.37
	ATOM	1111	CZ	PHE	445	17.460	5.015	26.113	1.00	30.37
	ATOM	1112	C	PHE	445	14.850	8.885	24.829	1.00	31.11
	ATOM	1113	Ō	PHE	445	15.924	8.947	24.221	1.00	32.20
	ATOM	1114	N	VAL	446	13.739	8.415	24.266	1.00	28.63
50	ATOM	1115	CA	VAL	446	13.787	7.943	22.889	1.00	27.94
	ATOM	1116	CB	VAL	446	12.478	7.193	22.478	1.00	28.48
	ATOM	1117	CG1	VAL	446	12.318	5.939	23.343	1.00	29.61
	ATOM	1118	CG2	VAL	446	11.265	8.092	22.607	1.00	27.23
	ATOM	1119	C	VAL	446	14.099	9.064	21.900	1.00	27.28
55	ATOM	1120	Õ	VAL	446	14.781	8.837	20.904	1.00	28.07
	ATOM	1121	N	CYS	447	13.619	10.275	20.904	1.00	28.97
	ATOM	1122	CA	CYS	447	13.819	11.394	21.272	1.00	29.14
	ATOM	1123	CB	CYS	447	13.919	12.653	21.693	1.00	28.90
	ATOM	1124	SG	CYS	447	11.389	12.633	21.309	1.00	35.68
60	ATOM	1125	C	CYS	447	15.420	11.677	21.309	1.00	28.03
	ATOM	1126	0	CYS	447	16.063	11.885	20.302	1.00	29.34
			_	J. 2 2	/	10.003	11.000	20.502	1.00	27.54

5	ATOM	1127	N	LEU	448	15.969	11.686	22.538	1.00	27.28
	ATOM	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	ATOM	1129	CB	LEU	448	17.733	11.932.	24.220	1.00	27.72
	ATOM	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
	ATOM	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
10	ATOM	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
	ATOM	1133	С	LEU	448	18.245	10.902	22.008	1.00	27.62
	ATOM	1134	0	LEU	448	19.207	11.252	21.327	1.00	25.10
	ATOM	1135	N	LYS	449	17.905	9.621	22.162	1.00	25.16
	ATOM	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55
15	ATOM	1137	CB	LYS	449	18.135	7.185	21.900	1.00	28.99
	ATOM	1138	CG	LYS	449	19.134	6.052	21.694	1.00	34.70
	ATOM	1139	CD	LYS	449	18.737	4.789	22.459	1.00	32.67
	ATOM	1140	CE	LYS	449	17.267	4.419	22.220	1.00	31.87
	ATOM	1141	NZ	LYS	449	17.022	2.967	22.472	1.00	29.14
20	ATOM	1142	C	LYS	449	18.626	8.749	19.990	1.00	25.88
	ATOM	1143	o	LYS	449	19.610	8.489	19.296	1.00	25.93
	ATOM	1144	N	SER	450	17.482	9.197	19.480	1.00	26.07
	ATOM	1145	CA	SER	450	17.323	9.421	18.052	1.00	27.24
	ATOM	1146	CB	SER	450	15.857	9.705	17.721	1.00	32.24
25	ATOM	1147	OG	SER	450	15.098	8.519	17.721	1.00	34.94
	ATOM	1148	C	SER	450	18.176	10.607	17.773	1.00	26.78
	ATOM	1149	0	SER	450	18.763	10.598	16.535		
	ATOM	1150	N	ILE	451	18.231	11.632	18.463	1.00	25.85
	ATOM	1151	CA	ILE	451	19.032				26.94
30	ATOM	1152	CB	ILE	451	18.950	12.810 13.850	18.155 19.291	1.00	26.13 27.72
50	ATOM	1153	CG2	ILE	451	20.019			1.00	
	ATOM	1154	CG1	ILE	451	17.553	14.929	19.101	1.00	20.53
	ATOM	1155	CD1	ILE	451	17.333	14.475	19.322	1.00	29.49
	ATOM	1156	C	ILE	451	20.489	15.473	20.447	1.00	36.24
35	ATOM	1157	0	ILE	451		12.381	17.989	1.00	24.88
55	ATOM	1158	N	ILE	452	21.161 20.977	12.771	17.034	1.00	26.96
	ATOM	1159	CA	ILE	452	20.377	11.582	18.931	1.00	22.72
	ATOM	1160	CB	ILE	452	22.660	11.120	18.880	1.00	21.95
	ATOM	1161	CG2	ILE	452		10.155	20.050	1.00	23.57
40	ATOM	1162	CG1	ILE	452	23.982	9.435	19.804	1.00	22.10
	ATOM	1163	CD1	ILE	452	22.718	10.949	21.371	1.00	21.70
	ATOM	1164	C	ILE	452	22.768	10.060	22.624	1.00	25.30
	ATOM		_			22.656	10.419	17.557	1.00	23.02
	ATOM	1165	N O	LEU	452 453	23.650	10.708	16.885	1.00	21.25
45	ATOM	1167	CA	LEU	453	21.779	9.497	17.173	1.00	22.83
1.5	ATOM	1168	CB	LEU	453	21.984	8.768	15.935	1.00	22.05
	ATOM	1169	CG			20.843	7.764	15.733	1.00	22.06
	ATOM	1170		LEU	453	20.712	7.189	14.324	1.00	22.03
			CD1	LEU	453	21.815	6.165	14.107	1.00	24.81
50	ATOM	1171	CD2	LEU	453	19.328	6.535	14.156	1.00	24.73
50	ATOM	1172	C	LEU	453	22.092	9.687	14.717	1.00	23.95
	ATOM	1173	0	LEU	453	22.962	9.501	13.860	1.00	24.60
	ATOM	1174	N	LEU	454	21.220	10.687	14.638	1.00	26.72
	ATOM	1175	CA	LEU	454	21.234	11.599	13.494	1.00	26.45
55	ATOM	1176	CB	LEU	454	19.852	12.242	13.330	1.00	25.51
55	ATOM	1177	CG	LEU	454	18.737	11.222	13.052	1.00	30.16
	ATOM	1178	CD1	LEU	454	17.405	11.926	12.955	1.00	28.76
	ATOM	1179	CD2	LEU	454	19.037	10.478	11.759	1.00	32.59
	ATOM	1180	С	LEU	454	22.292	12.703	13.552	1.00	28.24
66	ATOM	1181	0	LEU	454	22.778	13.148	12.513	1.00	29.06
60	ATOM	1182	N	ASN	455	22.638	13.146	14.757	1.00	26.56
	ATOM	1183	CA	ASN	455	23.604	14.236	14.934	1.00	26.79

5	ATOM	1184	CB	ASN	455	23.284	14.998	16.224	1.00	26.20
	MOTA	1185	CG	ASN	455	24.174	16.217	16.419	1.00	27.26
	MOTA	1186	OD1	ASN	455	24.171	17.134	15.602	1.00	30.83
	MOTA	1187	ND2	ASN	455	24.931	16.230	17.506	1.00	27.16
	ATOM	1188	С	ASN	455	25.062	13.782	14.954	1.00	30.63
10	MOTA	1189	0	ASN	455	25.965	14.517	14.525	1.00	27.69
	ATOM	1190	N	SER	456	25.268	12.569	15.461	1.00	30.48
	MOTA	1191	CA	SER	456	26.572	11.928	15.579	1.00	35.26
	ATOM	1192	CB	SER	456	26.393	10.393	15.505	1.00	39.69
	ATOM	1193	OG	SER	456	25.871	9.953	14.243	1.00	30.73
15	MOTA	1194	C	SER	456	27.627	12.344	14.562	1.00	35.56
	ATOM	1195	ō	SER	456	28.599	13.041	14.884	1.00	33.00
	ATOM	1196	N	GLY	457	27.437	11.886	13.334	1.00	33.88
	ATOM	1197	CA	GLY	457	28.393	12.189	12.292	1.00	
	ATOM	1198	C	GLY	457	27.876	13.017			36.77
20	ATOM	1199	0	GLY	457	28.310	12.805	11.136	1.00	37.02
	ATOM	1200	N	VAL	458	26.967		10.013	1.00	38.66
	ATOM	1201	CA	VAL	458		13.956	11.392	1.00	39.12
	ATOM	1202	CB	VAL		26.438	14.802	10.317	1.00	43.81
	ATOM	1202	CG1		458	25.231	15.648	10.755	1.00	44.25
25	ATOM	1204	CG2	VAL VAL	458	24.209	15.713	9.631	1.00	44.51
	ATOM	1205	C		458	24.638	15.098	12.013	1.00	50.53
	ATOM	1205	0	VAL	458	27.472	15.801	9.817	1.00	46.72
	ATOM	1207	N	VAL	458	27.391	16.265	8.681	1.00	47.08
	ATOM	1207	CA	TYR	459	28.432	16.144	10.670	1.00	50.74
30	ATOM	1208	CB	TYR	459	29.456	17.114	10.301	1.00	55.43
50	ATOM	1210	CG	TYR	459	29.647	18.129	11.433	1.00	56.62
	ATOM	1211		TYR	459	28.375	18.870	11.781	1.00	59.34
	ATOM	1211	CD1 CE1	TYR	459	28.094	19.229	13.095	1.00	60.73
	ATOM	1212		TYR	459	26.900	19.867	13.429	1.00	62.14
35	ATOM	1213	CD2	TYR	459	27.430	19.175	10.795	1.00	62.16
33	ATOM	1214	CE2 CZ	TYR	459	26.234	19.812	11.118	1.00	63.83
	ATOM	1215	OH	TYR	459	25.976	20.154	12.437	1.00	62.88
	ATOM	1217	C	TYR	459	24.790	20.764	12.767	1.00	62.56
	ATOM	1217	0	TYR	459	30.791	16.489	9.928	1.00	57.21
40	ATOM	1219	N	TYR	459	31.793	17.189	9.798	1.00	56.86
10	ATOM			THR	460	30.800	15.173	9.750	1.00	59.22
	ATOM	1220 1221	CA	THR	460	32.018	14.474	9.366	1.00	62.25
	ATOM		CB	THR	460	32.502	13.531	10.499	1.00	63.07
	ATOM	1222 1223	OG1	THR	460	33.474	12.613	9.983	1.00	67.80
45	ATOM	1223	CG2 C	THR	460	31.344	12.759	11.084	1.00	60.23
7.5	ATOM	1225		THR	460	31.759	13.678	8.086	1.00	63.54
	ATOM	1225	O N	THR	460	32.457	12.708	7.782	1.00	63.91
	ATOM		N	PHE	461	30.758	14.113	7.326	1.00	65.06
		1227	CA	PHE	461	30.395	13.446	6.080	1.00	67.00
50	ATOM	1228	CB	PHE	461	29.052	13.975	5.563	1.00	66.48
50	ATOM	1229	CG	PHE	461	27.867	13.147	5.991	1.00	66.30
	ATOM	1230	CD1	PHE	461	26.657	13.754	6.312	1.00	65.58
	ATOM	1231	CD2	PHE	461	27.963	11.760	6.085	1.00	66.41
	ATOM	1232	CE1	PHE	461	25.562	12.996	6.723	1.00	65.45
5.5	ATOM	1233	CE2	PHE	461	26.872	10.994	6.494	1.00	66.83
55	ATOM	1234	CZ	PHE	461	25.670	11.616	6.814	1.00	65.12
	ATOM	1235	С	PHE	461	31.463	13.604	5.004	1.00	68.38
	ATOM	1236	0	PHE	461	32.181	14.606	4.962	1.00	68.98
	ATOM	1237	N	LEU	462	31.542	12.601	4.132	1.00	69.57
60	ATOM	1238	CA	LEU	462	32.511	12.545	3.039	1.00	71.68
60	MOTA	1239	CB	LEU	462	32.080	11.475	2.030	1.00	71.00
	ATOM	1240	С	LEU	462	32.810	13.856	2.304	1.00	72.40
				•						

5	ATOM	1241	. 0	LEU	462	33.725	14.590	2.680	1.00	73.45
	ATOM	1242		SER	463	32.043	14.141	1.253		-
	ATOM	1243	CA	SER	463	32.262	15.343	0.449		
	ATOM	1244	CB	SER	463	32.544	14.942	-1.005		
	ATOM	1245	С	SER	463	31.126	16.362	0.491		
10	ATOM	1246	0	SER	463	30.455	16.528			
	ATOM	1247		SER	464	30.932		1.511		
	ATOM	1248		SER			17.049			
	ATOM	1249			464	29.892	18.063			
	ATOM			SER	464	30.514	19.457	-0.704		
15		1250		SER	464	29.108	17.887	-2.060	1.00	63.72
13	ATOM	1251		SER	464	28.657	18.862	-2.662	1.00	62.88
	ATOM	1252		THR	465	28.954	16.638	-2.493	1.00	60.93
	ATOM	1253		THR	465	28.205	16.343	-3.709	1.00	
	ATOM	1254	CB	THR	465	28.185	14.824	-4.004		
•	ATOM	1255	OG1	THR	465	27.525	14.135	-2.934		
20	ATOM	1256	CG2	THR	465	29.606	14.287	-4.149		
	ATOM	1257	С	THR	465	26.767	16.824	-3.523		
	ATOM	1258	0	THR	465	26.349	17.129	-2.407		
	ATOM	1259	N	LEU	466	26.013				·
	ATOM	1260	CA	LEU	466	24.625	16.892	-4.614		
25	ATOM	1261	CB	LEU	466		17.330	-4.550		
	ATOM	1262	CG	LEU	466	24.013	17.349	-5.956	1.00	
	ATOM	1263	CD1	LEU		22.953	18.415	-6.253	1.00	
	ATOM	1264			466	22.156	18.002	-7.482	1.00	
	ATOM		CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
30	ATOM	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
50		1266	0	LEU	466	22.961	16.845	-2.883	1.00	45.90
	ATOM	1267	N	LYS	467	24.093	15.099	-3.750	1.00	46.47
	ATOM	1268	CA	LYS	467	23.399	14.100	-2.947	1.00	47.45
	ATOM	1269	CB	LYS	467	23.802	12.693	-3.395	1.00	49.38
25	ATOM	1270	CG	LYS	467	22.829	11.602	-2.974	1.00	52.70
35	ATOM	1271	CD	LYS	467	23.561	10.301	-2.682	1.00	56.48
	ATOM	1272	CE	LYS	467	23.105	9.180	-3.604	1.00	59.54
	ATOM	1273	NZ	LYS	467	24.150	8.117	-3.732	1.00	61.22
	MOTA	1274	С	LYS	467	23.738	14.284	-1.472	1.00	46.89
	ATOM	1275	0	LYS	467	22.884	14.108	-0.604	1.00	46.06
40	ATOM	1276	N	SER	468	24.989	14.644	-1.202	1.00	
	ATOM	1277	CA	SER	468	25.457	14.854	0.160		45.82
	ATOM	1278	CB	SER	468	26.976	15.050		1.00	46.82
	ATOM	1279		SER	468	27.407	15.537	0.173	1.00	47.85
	ATOM	1280	C	SER	468	24.778		1.435	1.00	55.73
45	ATOM	1281	ō	SER	468		16.063	0.790	1.00	44.24
	ATOM	1282	N	LEU		24.473	16.062	1.983	1.00	42.98
	ATOM	1283	CA		469	24.547	17.100	-0.011	1.00	42.33
	ATOM	1284		LEU	469	23.890	18.301	0.486	1.00	40.42
	ATOM		CB	LEU	469	24.002	19.427	-0.545	1.00	44.47
50	ATOM	1285	CG	LEU	469	25.438	19.874	-0.849	1.00	46.70
50		1286	CD1	LEU	469	25.514	20.477	-2.246	1.00	46.70
	ATOM	1287	CD2	LEU	469	25.890	20.883	0.199	1.00	47.32
	ATOM	1288	C	LEU	469	22.423	17.996	0.786	1.00	39.06
	ATOM	1289	0	LEU	469	21.856	18.505	1.760	1.00	34.97
	ATOM	1290	N	GLU	470	21.814	17.151	-0.046	1.00	
55	ATOM	1291	CA	GLU	470	20.418	16.768	0.145	1.00	35.46
	ATOM	1292	CB	GLU	470	19.914	15.963			34.38
	ATOM	1293	CG	GLU	470	19.772		-1.052	1.00	38.02
	ATOM	1294	CD	GLU	470	19.772	16.773	-2.329	1.00	42.67
	ATOM	1295	OE1	GLU	470		15.923	-3.509	1.00	48.30
60	ATOM	1296	OE2	GLU		19.671	14.716	-3.538	1.00	50.53
	ATOM	1297	C		470	18.666	16.463	-4.412	1.00	51.06
		<i>31</i>		GLU	470	20.290	15.916	1.403	1.00	34.37

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_			_	GT 11	470	19.321	16.035	2.157	1.00	32.60
5	ATOM	1298	0	GLU			15.046	1.606	1.00	34.66
	MOTA	1299	N	GLU	471	21.274		2.766	1.00	35.68
	MOTA	1300	CA	GLU	471	21.309	14.162		1.00	34.57
	ATOM	1301	CB	GLU	471	22.515	13.222	2.671	1.00	37.98
	MOTA	1302	CG	GLU	471	22.376	12.122	1.614		
10	MOTA	1303	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
	ATOM	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12
	ATOM	1305	OE2	GLU	471	21.974	10.061	2.737	1.00	32.11
	ATOM	1306	C	GLU	471	21.393	14.983	4.052	1.00	34.79
	ATOM	1307	Ō	GLU	471	20.596	14.793	4.969	1.00	32.80
1.5		1308	N	LYS	472	22.358	15.898	4.112	1.00	33.93
15	ATOM	1308	CA	LYS	472	22.518	16.739	5.291	1.00	35.58
	ATOM			LYS	472	23.683	17.710	5.097	1.00	39.11
	ATOM	1310	CB			25.050	17.050	5.138	1.00	41.47
	ATOM	1311	CG	LYS	472	26.080	17.957	5.794	1.00	46.97
	ATOM	1312	CD	LYS	472		17.286	5.862	1.00	48.40
20	MOTA	1313	CE	LYS	472	27.445			1.00	51.55
	MOTA	1314	NZ	LYS	472	27.850	16.702	4.547		
	ATOM	1315	С	LYS	472	21.237	17.523	5.582	1.00	34.78
	ATOM	1316	0	LYS	472	20.795	17.607	6.724	1.00	33.95
	ATOM	1317	N	ASP	473	20.643	18.097	4.545	1.00	33.47
25	ATOM	1318	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
	ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
	ATOM	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24
	ATOM	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
	ATOM	1322	OD2	ASP	473	17.750	21.396	3.932	1.00	45.59
30	ATOM	1323		ASP	473	18.339	17.998	5.338	1.00	32.93
30	ATOM	1324		ASP	473	17.642	18.416	6.264	1.00	32.87
		1325		HIS	474	18.199	16.784	4.827	1.00	32.74
	ATOM	1325		HIS	474	17.185	15.882	5.343	1.00	32.21
	ATOM			HIS	474	17.185	14.575	4.568	1.00	32.79
2.5	MOTA	1327		HIS	474	16.047	13.675	4.924	1.00	36.22
35	MOTA	1328				14.711	13.813	4.750	1.00	38.33
	ATOM	1329		HIS	474		12.456	5.542	1.00	38.97
	MOTA	1330		HIS	474	16.227	11.883	5.732	1.00	37.99
	MOTA	1331		HIŞ	474	15.053		5.261	1.00	37.43
	ATOM	1332		HĮS	474	14.116	12.686	6.815	1.00	29.74
40	ATOM	1333		HIS	474	17.403	15.573		1.00	29.90
	ATOM	1334		HIS	474	16.460	15.543	7.596		27.80
	MOTA	1335		ILE	475	18.653	15.326	7.185	1.00	
	MOTA	1336	CA	ILE	475	18.971	15.014	8.571	1.00	25.61
	ATOM	1337	7 CB	ILE	475	20.478	14.708	8.720	1.00	25.59
45	ATOM	1338	CG2	ILE	475	20.877		10.193	1.00	27.17
	MOTA	1339	CG1	ILE	475	20.787	13.341	8.092	1.00	26.17
	ATOM	1340	CD1	ILE	475	22.258	13.071	7.849		27.07
	MOTA	1341	L C	ILE	475	18.576	16.201	9.460		27.91
	MOTA	1342	2 0	ILE	475	17.928	16.038	10.485		29.16
50	ATOM	1343		HIS	476	18.956	17.404	9.054	1.00	
20	ATOM	1344		HIS	476	18.621		9.846	1.00	29.73
	ATOM	1345		HIS	476	19.342		9.281	1.00	32.27
	ATOM	1346		HIS	476	20.777		9.699		39.44
					476	21.355		10.915		
	ATOM	1347			476	21.809		8.808		
55	MOTA	1348						9.456		
	ATOM	1349			476	22.959		10.735		_
	ATOM	1350			476	22.712				
	MOTA	135		HIS	476	17.120		9.948		
	MOTA	135		HIS		16.636		10.951		
60	MOTA	135	3 N	ARG		16.374		8.929		
	MOTA	135	4 CA	ARG	477	14.929	18.570	8.956	1.00	31.53

5	ATOM	135	5 CB	אפע	477	74 747				•
	ATOM	135		ARG ARG		14.343				
	ATOM	135				14.425				40.46
	ATOM	135		ARG		13.698			1.00	45.22
	ATOM	135		ARG		14.107				53.05
10	ATOM	136	-	ARG		13.647		4.376	1.00	55.89
	ATOM					12.756		5.274	1.00	56.17
	ATOM	136			477	14.084		3.457	1.00	59.49
	ATOM	136		ARG	477	14.310	17.582	9.931	1.00	
		136		ARG	477	13.360		10.649	1.00	
15	ATOM	136		VAL	478	14.863	16.375	9.972		
13	ATOM	136		VAL	478	14.351	15.369	10.887		
	MOTA	136		VAL	478	14.937	13.975	10.575		
	ATOM	136			478	14.461	12.973	11.609	_	
	ATOM	1368		VAL	478	14.506		9.169		31.00
20	ATOM	1369		VAL	478	14.696	15.774	12.316		29.81
20	MOTA	1370		VAL	478	13.860	15.677	13.220		30.25
	MOTA	137	LN	LEU	479	15.929	16.232	12.516	1.00	
	ATOM	1372	CA	LĘU	479	16.360	16.674	13.836	1.00	28.81
	ATOM	1373	CB	LEU	479	17.799	17.210	13.779	1.00	28.74
	ATOM	1374		LEU	479	18.910	16.152	13.853	1.00	26.65
25	ATOM	1375	CD1	LEU	479	20.231	16.772	13.395		26.05
	ATOM	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.81
	ATOM	1377	7 C	LEU	479	15.411	17.777	14.313	1.00	25.34
	ATOM	1378	0	LEU	479	14.997	17.786	15.472	1.00	29.54
	ATOM	1379	N	ASP	480	15.076	18.703		1.00	29.00
30	ATOM	1380	CA	ASP	480	14.162	19.800	13.415	1.00	31.52
	ATOM	1381	CB	ASP	480	13.943	20.712	13.741	1.00	33.84
	ATOM	1382		ASP	480	15.055	21.743	12.528	1.00	34.37
	ATOM	1383		ASP	480	15.119	22.354	12.345	1.00	36.26
	ATOM	1384		ASP	480	15.860	22.354	11.257	1.00	36.56
35	ATOM	1385		ASP	480	12.818	19.222	13.274	1.00	34.19
	ATOM	1386		ASP	480	12.186		14.174	1.00	33.48
	ATOM	1387		LYS	481	12.100	19.724	15.105	1.00	33.89
	ATOM	1388		LYS	481	11.106	18.161	13.498	1.00	33.90
	ATOM	1389		LYS	481	10.719	17.536	13.839	1.00	32.97
40	ATOM	1390		LYS	481		16.489	12.784	1.00	34.66
	ATOM	1391		LYS	481	11.164	16.895	15.225	1.00	33.57
	ATOM	1392	N	ILE	482	10.167	16.869	15.943	1.00	35.37
	ATOM	1393	CA	ILE		12.328	16.377	15.607	1.00	32.71
	ATOM	1394		ILE	482 482	12.457	15.764	16.922	1.00	31.60
45	ATOM	1395	CG2	ILE		13.743	14.913	17.028	1.00	32.65
•	ATOM	1396	CG1	ILE	482	13.877	14.338	18.430	1.00	32.50
	ATOM	1397	CD1	•	482	13.697	13.785	15.995	1.00	32.72
	ATOM	1398	CDI	ILE	482	14.978	12.969	15.908	1.00	33.37
	ATOM	1399		ILE	482	12.456	16.853	17.994	1.00	31.69
50	ATOM	1400	0	ILE	482	11.946	16.649	19.097	1.00	29.98
•	ATOM	1400	N	THR	483	13.027	18.012	17.679	1.00	31.33
	ATOM		CA	THR	483	13.022	19.109	18.644	1.00	31.71
	ATOM	1402	CB	THR	483	13.756	20.351	18.109	1.00	32.92
		1403	OG1	THR	483	15.111	20.012	17.788	1.00	29.99
55	ATOM	1404	CG2	THR	483	13.756	21.452	19.160	1.00	30.47
رر	ATOM	1405	C	THR	483	11.559	19.483	18.920	1.00	32.85
	ATOM	1406	0	THR	483	11.146	19.598	20.070		31.83
	ATOM	1407	N	ASP	484	10.785	19.656	17.851		31.83
	ATOM	1408	CA	ASP	484	9.369	20.003	17.965		
	ATOM	1409	CB	ASP	484	8.708	20.013	16.591		34.15
60	ATOM	1410	CG	ASP	484	9.270	21.080	15.680		37.41
	ATOM	1411	OD1	ASP	484	9.871	22.045			42.02
					_	2.0,1	22.03	16.198	1.00	43.26

5	MOTA	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49 33.16
	ATOM	1413	С	ASP	484	8.657	18.985	18.840	1.00	34.86
	MOTA	1414	0	ASP	484	7.830	19.339	19.676	1.00	33.91
	MOTA	1415	N	THR	485	8.996	17.715	18.646 19.414	1.00	34.41
	ATOM	1416	CA	THR	485	8.396	16.635	18.885	1.00	33.58
10	MOTA	1417	CB	THR	485	8.875	15.268	17.542	1.00	37.04
	MOTA	1418	OG1	THR	485	8.400	15.094	19.751	1.00	30.89
	MOTA	1419	CG2	THR	485	8.347	14.138	20.903	1.00	35.15
	MOTA	1420	C	THR	485	8.708	16.757	21.744	1.00	31.99
	MOTA	1421	0	THR	485	7.818	16.600 17.046	21.744	1.00	33.77
15	MOTA	1422	N	LEU	486	9.966	17.192	22.621	1.00	34.31
	MOTA	1423	CA	LEU	486	10.368	17.192	22.721	1.00	32.00
	MOTA	1424	CB	LEU	486	11.879	16.201	22.754	1.00	34.99
	ATOM	1425	CG	LEU	486	12.776	16.613	22.521	1.00	32.65
	ATOM	1426	CD1	LEU	486	14.233	15.481	24.105	1.00	29.90
20	ATOM	1427	CD2	LEU	486	12.635 9.597	18.348	23.256	1.00	34.87
	MOTA	1428	C	LEU	486	9.078	18.225	24.362	1.00	35.85
	ATOM	1429	0	LEU	486 487	9.513	19.469	22.548	1.00	35.59
	ATOM	1430	N	ILE	487	8.787	20.625	23.064	1.00	36.79
25	MOTA	1431	CA CB	ILE ILE	487	8.890	21.826	22.095	1.00	37.32
25	MOTA	1432 1433	CG2	ILE	487	7.833	22.884	22.443	1.00	40.19
	ATOM	1434	CG1	IĻĘ	487	10.292	22.443	22.181	1.00	36.00
	ATOM ATOM	1435	CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
	ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56
30	ATOM	1437	0	ILE	487	6.708	20.628	24.282	1.00	38.52
30	ATOM	1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
	ATOM	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
	ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
	ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
35	ATOM	1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
	ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
	ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
	MOTA	1445	NE2	HIS	488	1.477	17.144	21.385	1.00	50.22
	ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
40	MOTA	1447	0	HIS	488	4.233	18.498	24.467	1.00	43.02
	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	39.91
	MOTA	1449	CA	LEU	489	5.936	16.399	25.048	1.00	39.93
	MOTA	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
	ATOM	1451		LEU	489	6.961	14.242	24.056	1.00	39.31
45	MOTA	1452		LEU	489	8.259	13.456	24.027	1.00	39.01
	ATOM	1453		LEU	489	5.799	13.345	24.459	1.00	41.98
	MOTA	1454		LEU	489	5.973	17.203	26.339	1.00	40.24 38.72
	MOTA	1455		LEU	489	5.267	16.888	27.298	1.00	
	ATOM	1456		MET	490	6.798	18.246	26.353	1.00	
50	ATOM	1457		MET	490	6.939	19.102	27.522	1.00	
	ATOM	1458		MET	490	8.208	19.953	27.394	1.00	
	MOTA	1459		MET	490	9.495	19.169	27.608		
	ATOM	1460		MET	490	10.978	20.106	27.161		
	MOTA	1461		MET	490	12.178	18.775	27.056		
55	MOTA	1462		MET	490	5.718	20.004	27.717 28.848		
	ATOM	1463		MET	490	5.296	20.258	26.616		
	ATOM	1464		ALA	491	5.162		26.693		
	MOTA	1465		ALA	491	3.983	21.351 21.879	25.311		
	ATOM	1466		ALA	491	3.622 2.841		27.251		
60	MOTA	1467		ALA	491			28.095		
	ATOM	1468	30	ALA	491	2.073	20.96/	20.093	1.00	

5	MOTA	1469	N	LYS	492	2.752	19.268	26.783	1.00	46.29
	MOTA	1470	CA	LYS	492	1.711	18.351	27.222	1.00	49.90
	ATOM	1471	CB	LYS	492	1.772	17.053	26.411	1.00	50.03
	MOTA	1472	CG	LYS	492	1.087	17.135	25.062	1.00	53.81
	ATOM	1473	CD	LYS	492	-0.002	16.084	24.930	1.00	59.00
10	ATOM	1474	CE	LYS	492	-0.988	16.453	23.827	1.00	61.85
	ATOM	1475	NZ	LYS	492	-1.351	15.281	22.976	1.00	62.89
	ATOM	1476	С	LYS	492	1.841	18.025	28.701	1.00	51.15
	ATOM	1477	0	LYS	492	0.845	17.784	29.379	1.00	53.37
	ATOM	1478	N	ALA	493	3.072	18.012	29.199	1.00	50.15
15	ATOM	1479	CA	ALA	493	3.321	17.706	30.600	1.00	49.17
	ATOM	1480	CB	ALA	493	4.777	17.314	30.794	1.00	50.39
	ATOM	1481	С	ALA	493	2.971	18.885	31.501	1.00	49.36
	ATOM	1482	0	ALA	493	3.089	18.799	32.723	1.00	51.57
	ATOM	1483	N	GLY	494	2.554	19.989	30.893	1.00	48.61
20	ATOM	1484	CA	GLY	494	2.185	21.159	31.671	1.00	46.92
	ATOM	1485	C	GLY	494	3.322	22.107	32.006	1.00	45.46
	ATOM	1486	0	GLY	494	3.206	22.921	32.919	1.00	43.58
	ATOM	1487	N	LEU	495	4.431	22.009	31.284	1.00	44.81
	ATOM	1488	CA	LEU	495	5.555	22.899	31.540	1.00	42.34
25	ATOM	1489	CB	LEU	495	6.847	22.293	30.988	1.00	43.79
	ATOM	1490	CG	LEU	495	7.712	21.459	31.936	1.00	40.99
	ATOM	1491	CD1	LEU	495	7.022	20.156	32.260	1.00	44.70
	ATOM	1492	CD2	LEU	495	9.072	21.189	31.270	1.00	42.12
	ATOM	1493	C	LEU	495	5.278	24.227	30.847	1.00	42.12
30	ATOM	1494	ō	LEU	495	4.664	24.258	29.778	1.00	42.13
	MOTA	1495	N	THR	496	5.718	25.324	31.452	1.00	42.73
	MOTA	1496	CA	THR	496	5.521	26.636	30.845	1.00	43.56
	ATOM	1497	CB	THR	496	5.841	27.767	31.829	1.00	46.09
	ATOM	1498	OG1	THR	496	7.222	27.688	32.208	1.00	43.92
35	ATOM	1499	CG2	THR	496	4.965	27.662	33.064	1.00	45.63
	ATOM	1500	С	THR	496	6.471	26.764	29.660	1.00	45.54
	ATOM	1501	O	THR	496	7.370	25.939	29.488	1.00	43.39
	ATOM	1502	N	LEU	497	6.280	27.800	28.849	1.00	45.02
	MOTA	1503	CA	LEU	497	7.135	28.020	27.688	1.00	45.12
40	ATOM	1504	CB	LEU	497	6.710	29.286	26.944	1.00	46.62
	ATOM	1505	CG	LEU	497	5.933	29.080	25.640	1.00	50.20
	ATOM	1506	CD1	LEU	497	5.886	30.397	24.875	1.00	50.25
	ATOM	1507	CD2	LEU	497	6.589	27.990	24.798	1.00	50.91
	ATOM	1508	С	LEU	497	8.599	28.135	28.101	1.00	44.94
45	ATOM	1509	0	LEU	497	9.474	27.516	27.493	1.00	45.03
	ATOM	1510	N	GLN	498	8.862	28.927	29.137	1.00	41.14
	ATOM	1511	CA	GLN	498	10.221	29.101	29.627	1.00	40.54
	ATOM	1512	CB	GLN	498	10.246	30.140	30.743	1.00	43.82
	ATOM	1513	CG	GLN	498	11.585	30.270	31.437	1.00	43.37
50	ATOM	1514	CD	GLN	498	11.539	31.260	32.584	1.00	47.03
	ATOM	1515	OE1	GLN	498	10.565	31.308	33.332	1.00	49.18
	ATOM	1516	NE2	GLN	498	12.591	32.054	32.727	1.00	45.30
	ATOM	1517	С	GLN	498	10.777	27.773	30.145	1.00	39.39
	ATOM	1518	0	GLN	498	11.923	27.422	29.866	1.00	35.05
55	ATOM	1519	N	GLN	499	9.965	27.040	30.902	1.00	36.49
	ATOM	1520	CA	GLN	499	10.391	25.748	31.434	1.00	36.49
	ATOM	1521	CB	GLN	499	9.314	25.155	32.344	1.00	
	ATOM	1522	CG	GLN	499	9.155	25.825	33.703	1.00	38.84 41.33
	ATOM	1523	CD	GLN	499	8.039	25.823	34.512	1.00	
60	ATOM	1524	OE1	GLN	499	7.027		33.955	1.00	42.74 45.44
	ATOM	1525	NE2	GLN	499	8.222	25.107	35.829		
	•					0.222	23.107	22.023	1.00	43.48

5	ATOM	1526	С	GLN	499	10.655	24.773	30.285	1.00	35.03
,	ATOM	1527	0	GLN	499	11.446	23.832	30.422	1.00	36.59
	ATOM	1528	И	GLN	500	9.980	24.994	29.162	1.00	34.14
		1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
	ATOM		CB	GLN	500	9.042	24.436	26.958	1.00	33.90
10	ATOM	1530		GLN	500	7.672	23.872	27.315	1.00	36.62
10	ATOM	1531	CG		500	6.558	24.419	26.435	1.00	40.17
	ATOM	1532	CD	GLN		6.660	24.417	25.207	1.00	40.22
	MOTA	1533	OE1	GLN	500	5.482	24.417	27.064	1.00	41.82
	ATOM	1534	NE2	GLN	500			27.358	1.00	34.96
	ATOM	1535	C	GLN	500	11.511	24.350	27.124	1.00	30.79
15	ATOM	1536	0	GLN	500	12.256	23.387		1.00	34.21
	MOTA	1537	N	HIS	501	11.835	25.612	27.078	1.00	37.42
	MOTA	1538	CA	HIS	501	13.117	25.966	26.480		43.08
	MOTA	1539	CB	HIS	501	13.195	27.476	26.246	1.00	
	MOTA	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
20	MOTA	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
	ATOM	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
	MOTA	1543	CE1	HIS	501	10.325	29.337	25.037	1.00	54.36
	ATOM	1544	NE2	HĮS	501	10.466	28.508	24.018	1.00	55.19
	ATOM	1545	С	HIS	501	14.255	25.543	27.395	1.00	35.79
25	MOTA	1546	0	HIS	501	15.271	24.996	26.945	1.00	36.20
	MOTA	1547	N	GLN	502	14.086	25.799	28.685	1.00	33.90
	MOTA	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
	MOTA	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
	ATOM	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
30	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
	ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
	ATOM	1554	С	GĻŅ	502	15.340	23.932	29.716	1.00	31.79
	ATOM	1555	0	GLN	502	16.483	23.479	29.769	1.00	28.00
35	MOTA	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
	ATOM	1557		ARG	503	14.436	21.704	29.779	1.00	29.91
	ATOM	1558		ARG	503	13.107	21.011	30.052	1.00	32.79
	ATOM	1559		ARG	503	13.258	19.541	30.400	1.00	30.84
	ATOM	1560		ARG	503	11.930	18.935	30.798	1.00	30.61
40	ATOM	1561		ARG	503	12.021	17.490	30.992	1.00	28.50
	ATOM	1562		ARG	503	12.489	16.908	32.093	1.00	29.00
	ATOM	1563		ARG	503	12.917	17.640	33.114	1.00	29.85
	ATOM	1564		ARG	503	12.512	15.583	32.180	1.00	33.73
	ATOM	1565		ARG	503	15.051	21.152	28.496	1.00	29.89
45	ATOM	1566		ARG	503	15.895	20.259	28.548	1.00	29.69
,,,	ATOM	1567		LEU	504	14.624	21.675	27.351	1.00	28.99
	ATOM	1568		LEU	504	15.164	21.223	26.075	1.00	28.90
	ATOM	1569		LEU	504	14.566	22.023	24.916	1.00	27.72
	ATOM	1570		LEU	504	15.327	21.901	23.593	1.00	30.47
50	ATOM	1571		LEU	504	15.252	20.453	23.117		31.74
50	ATOM	1572		LEU	504	14.742	22.843	22.542	1.00	
		1573		LEU	504	16.681	21.419	26.089	1.00	
	ATOM			LEU	504	17.439	20.536	25.672	1.00	26.38
	MOTA	1574			505	17.439	22.585	26.564		28.51
55	ATOM	1575		ALA			22.899	26.632	1.00	25.98
55	ATOM	1576		ALA	505	18.535		27.039		29.86
	ATOM	1577		ALA	505	18.735		27.604		
	ATOM	1578		ALA	505	19.261	21.977	27.804		
	ATOM	1579		ALA	505	20.340	21.462			
	ATOM	1580		GLN	506	18.677	21.771	28.784		
60	ATOM	1581		GLN	506	19.299	20.907			
	ATOM	1582	2 CB	GLN	506	18.434	20.796	31.043	1.00	۵1.15

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5	MOTA	1583	CG	GLN	506	18.414	22.027 22.116	31.945	1.00	32.48 38.40
	MOTA	1584	CD	GLN	506	17.111		32.736 32.754	1.00	35.97
	ATOM	1585	OE1	GLN	506	16.319 16.879	21.167 23.257	33.386	1.00	38.07
	ATOM	1586	NE2	GLN	506	19.500	19.509	29.217	1.00	24.53
10	MOTA	1587	C	GLN	506	20.536	18.889	29.441	1.00	26.42
10	MOTA	1588	O N	GLN	506 507	18.505	19.017	28.484	1.00	26.78
	MOTA	1589 1590	N CA	LEU	507	18.578	17.678	27.902	1.00	26.18
	MOTA	1591	CB	LEU	507	17.225	17.286	27.295	1.00	31.48
	ATOM	1591	CG	LEU	507	16.052	16.961	28.231	1.00	32.59
15	ATOM ATOM	1593	CD1	LEU	507	14.836	16.561	27.389	1.00	33.78
13	ATOM	1594	CD2	LEU	507	16.431	15.838	29.174	1.00	30.18
	MOTA	1595	C	LEU	507	19.652	17.583	26.819	1.00	26.03
	ATOM	1596	0	LEU	507	20.421	16.621	26.771	1.00	27.28
	ATOM	1597	N	LEU	508	19.713	18.583	25.950	1.00	24.31
20	ATOM	1598	CA	LEU	508	20.690	18.557	24.863	1.00	23.68
20	ATOM	1599	CB	LEU	508	20.339	19.629	23.828	1.00	23.91
	ATOM	1600	CG	LEU	508	19.004	19.436	23.102	1.00	24.68
	ATOM	1601	CD1	LEU	508	18.905	20.416	21.945	1.00	25.11
	ATOM	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	27.53
25	ATOM	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.93
20	ATOM	1604	ō	LEU	508	23.062	18.200	24.736	1.00	21.36
	ATOM	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
	ATOM	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
	ATOM	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
30	ATOM	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
20	ATOM	1609	CD1	LEU	509	23.529	23.114	28.921	1.00	35.23
	ATOM	1610	CD2	LEU	509	24.818	22.525	26.856	1.00	30.48
	MOTA	1611	C	LEU	509	24.154	18.327	27.540	1.00	26.08
	ATOM	1612	0	LEU	509	25.354	18.068	27.547	1.00	23.92
35	ATOM	1613	N	ILE	510	23.254	17.462	27.993	1.00	24.60
	ATOM	1614	CA	ILE	510	23.712	16.172	28.496	1.00	25.12
	ATOM	1615	CB	ILE	510	22.568	15.368	29.161	1.00	28.51
	ATOM	1616	CG2	ILE	510	23.051	13.965	29.506	1.00	31.67
	ATOM	1617	CG1	ΙĻΕ	510	22.141	16.060	30.459	1.00	31.18
40	ATOM	1618	CD1	ILE	510	20.712	15.749	30.882	1.00	37.16
	ATOM	1619	С	ILE	510	24.337	15.351	27.364	1.00	23.86
	ATOM	1620	0	ILE	510	25.225	14.534	27.600	1.00	24.14
	ATOM	1621	N	LEU	511	23.889	15.586	26.133	1.00	25.10
	ATOM	1622	CA	LEU	511	24.420	14.862	24.977	1.00	25.63
45	ATOM	1623	CB	LEU	511	23.628	15.225	23.714	1.00	23.89
	ATOM	1624	CG	LEU	511	22.152	14.801	23.659	1.00	25.78
	ATOM	1625	CD1	LEU	511	21.648	14.920	22.224	1.00	26.55
	ATOM	1626	CD2	LEU	511	21.990	13.363	24.146	1.00	26.29
	ATOM	1627	C	LEU	511	25.912	15.152	24.771	1.00	27.10
50	ATOM	1628	0	LEU	511	26.641	14.332	24.214	1.00	24.98
	ATOM	1629	N	SER	512	26.372	16.319	25.213	1.00	24.75
	ATOM	1630	CA	SER	512	27.787	16.637	25.076	1.00	23.68
	MOTA	1631	CB	SER	512	28.023	18.129	25.358	1.00	26.12
	ATOM	1632	OG	SER	512	29.271	18.327	25.986	1.00	37.17
55	ATOM	1633	С	SER	512	28.594	15.765	26.050	1.00	23.15
	ATOM	1634	0	SER	512	29.742	15.383	25.769	1.00	22.15
	ATOM	1635	N	AHIS	513	27.993	15.456	27.192	0.50	21.53
	ATOM	1636	N	BHIS	513	28.008	15.453	27.202	0.50	20.99
	ATOM	1637	CA	AHIS	513	28.645	14.624	28.196	0.50	21.79
60	ATOM	1638	CA	BHIS	513	28.696	14.607	28.174		20.94
	ATOM	1639	CB	AHIS	513	27.920	14.776	29.536	0.50	23.59

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5	ATOM	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
	ATOM	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
	ATOM	1643	CD2	AHIS	513	29.223	16.616	30.824	0.50	27.56
	ATOM	1644	CD2	BHIS	513	30.095	14.211	31.001	0.50	24.22
10	ATOM	1645	ND1	AHIS	513	27.204	17.117	30.160	0.50	30.62
	MOTA	1646	ND1	BHIS	513	28.285	13.105	31.523	0.50	27.00
	ATOM	1647	CE1	AHIS	513	27.693	18.185	30.763	0.50	26.32
	ATOM	1648	CE1	BHIS	513	29.225	12.740	32.376	0.50	24.40
	ATOM	1649	NE2	AHIS	513	28.916	17.908	31.176	0.50	28.30
15	ATOM	1650	NE2	BHIS	513	30.334	13.396	32.081	0.50	25.54
	MOTA	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	ATOM	1652	C	BHIS	513	28.720	13.171	27.738	0.50	19.42
	ATOM	1653	0	AHIS	513					
	ATOM	1654	0	BHIS		29.601	12.426	28.026	0.50	22.45
20	ATOM	1655	N		513	29.707	12.457	27.809	0.50	22.62
20	ATOM	1656	CA	ILE	514	27.633	12.753	27.015	1.00	20.76
				ILE	514	27.572	11.396	26.492	1.00	20.94
	ATOM	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
	ATOM	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
25	ATOM	1659	CG1	ILE	514	25.185	10.965	27.139	1.00	27.91
23	ATOM	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	ATOM	1661	C	IĻE	514	28.641	11.256	25.398	1.00	20.66
	ATOM	1662	0	ILE	514	29.298	10.226	25.285	1.00	22.21
	ATOM	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
30	ATOM	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
30	ATOM	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	ATOM	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
	ATOM	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55
	ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24
35	ATOM	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
33	ATOM	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
	ATOM	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
	ATOM ATOM	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
		1673	0	ARG	515	32.068	11.305	23.795	1.00	20.06
40	ATOM	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
40	ATOM	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
	ATOM ATOM	1676	CB	HIS	516	32.566	13.794	27.206	1.00	24.03
		1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
	ATOM	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
45	ATOM ATOM	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
73	ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
	ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
		1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
	ATOM	1683	0	HIS	516	34.059	10.852	26.362	1.00	23.66
50	ATOM	1684	N	MEŢ	517	31.969	10.786	27.168	1.00	20.91
50	ATOM	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
	ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
	ATOM	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
	ATOM	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
55	ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
33	ATOM	1690	C	MET	517	32.399	8.448	26.564	1.00	23.26
	ATOM	1691	0	MET	517	33.213	7.547	26.728	1.00	26.08
	ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
	ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
60	ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
60	ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
	MOTA	1696	С	SER	518	33.432	7.862	23.810	1.00	25.15

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5	ATOM	1697	0	SER	518	34.111	6.866	23.532	1.00	22.94
	ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	
	ATOM	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
	ATOM	1700	CB	ASN	519	35.605	10.807	23.157	1.00	24.46
	ATOM	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
10	ATOM	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
	ATOM	1703	ND2		519	34.459	12.715	22.224	1.00	28.81
	ATOM	1704	С	ASN	519	36.292	8.643	24.201	1.00	21.46
	ATOM	1705	0	ASN	519	37.251	8.015	23.752		
	ATOM	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.56
15	ATOM	1707	CA	LYS	520	36.964	8.171		1.00	23.23
	ATOM	1708	СВ	LYS	520	36.581		26.488	1.00	26.35
	ATOM	1709	CG	LYS	520		8.592	27.912	1.00	27.53
	ATOM	1710	CD	LYS		36.618	10.101	28.174	1.00	33.74
	ATOM	1711	CE		520	37.962	10.710	27.811	1.00	42.09
20	ATOM	1711	NZ	LYS	520	39.047	10.307	28.802	1.00	43.97
20	ATOM	1713		LYS	520	39.858	11.480	29.254	1.00	48.07
	ATOM		С	LYS	520	36.899	6.644	26.376	1.00	27.71
		1714	0	LYS	520	37.913	5.957	26.501	1.00	27.15
	ATOM	1715	N	GLY	521	35.704 [.]	6.117	26.141	1.00	25.02
25	ATOM	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
23	ATOM	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
	ATOM	1718	0	GLY	521	36.924	3.128	24.775	1.00	26.84
	ATOM	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
	ATOM	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
20	MOTA	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
30	ATOM	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
	ATOM	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
	ATOM	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
	ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
~ -	MOTA	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70
35	ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
	ATOM	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
	ATOM	1729	CE	AMĘT	522	33.142	4.017	19.031	0.50	31.29
	MOTA	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
	ATOM	1731	С	AMET	522	38.242	4.532	22.512	0.50	28.99
40	ATOM	1732	С	BMET	522	38.224	4.567	22.483	0.50	30.76
	ATOM	1733	0	AMET	522	38.939	3.743	21.870	0.50	31.65
	ATOM	1734	0	BMET	522	38.905	3.793	21.807	0.50	32.87
	ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
	ATOM	1736	CA	GĻŪ	523	40.190	5.576	23.524	1.00	34.09
45	ATOM	1737	CB	GLU	523	40.515	6.725	24.480	1.00	35.59
	ATOM	1738	CG	GĻŲ	523	40.658	8.079	23.784		
	ATOM	1739	CD	GĻŪ	523	40.560	9.265	24.739	1.00	43.35
	ATOM	1740	OE1	GĻŲ	523	39.832			1.00	46.63
	ATOM	1741	OE2	GĻU	523		10.240	24.416	1.00	47.64
50	ATOM	1742	C	GLU	523	41.212	9.225	25.805	1.00	43.09
	ATOM	1743	0	GLU		40.718	4.260	24.061	1.00	34.62
	ATOM	1744			523	41.733	3.747	23.596	1.00	
	ATOM	1745	N	HIS	524	40.021	3.700	25.042	1.00	36.33
			CA	HIS.	524	40.455	2.427	25.607	1.00	39.20
55	ATOM	1746	CB	HIS.	524	39.678	2.093	26.878	1.00	40.75
))	ATOM	1747	CG	HIS_	524	40.061	0.774	27.473	1.00	48.10
	ATOM	1748	CD2	HIS	524	41.192	0.376	28.104	1.00	48.56
	ATOM	1749	ND1	HIS	524	39.247	-0.338	27.412	1.00	48.84
	MOTA	1750	CE1	HIS	524	39.859	-1.362	27.978	1.00	50.19
	ATOM	1751	NE2	HIS	524	41.041	-0.956	28.407	1.00	51.61
60	MOTA	1752	С	HIS	524	40.290	1.282	24.613	1.00	38.06
	ATOM	1753	0	HIS	524	41.226	0.521	24.371	1.00	38.18
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5	3 moss	1754			505	20 101		24 224		26.06
5	ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
	ATOM	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
	ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
	ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
10	ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
10	ATOM	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
	ATOM	1760	C	LEU	525	39.859	0.057	21.954	1.00	41.32
	ATOM	1761	0	LEU	525	40.244	-1.015	21.487	1.00	40.76
	ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
. ~	ATOM	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00
15	ATOM	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
	ATOM	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
	ATOM	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	MOTA	1767	CE1	TYR	526	42.681	2.875	16.305	1.00	61.21
	ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
20	MOTA	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
	MOTA	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
	MOTA	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	MOTA	1772	С	TYR	526	42.671	0.871	20.964	1.00	50.14
	ATOM	1773	0	TYR	526	43.471	0.303	20.223	1.00	50.73
25	MOTA	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
	MOTA	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
	MOTA	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	MOTA	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
20	MOTA	1778	С	SER	527	44.365	-0.718	23.054	1.00	60.39
30	MOTA	1779	0	SER	527	45.398	-1.185	23.534	1.00	60.43
	MOTA	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
	ATOM	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	MOTA	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
2.5	ATOM	1783	CG	MEŢ	528	41.237	-2.606	24.222	1.00	70.10
35	MOTA	1784	SD	MET	528	39.895	-3.569	24.983	1.00	71.70
	ATOM	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
	ATOM	1786	C	MET	528	42.726	-3.502	21.513	1.00	70.33
	ATOM	1787	0	MET	528	42.170	-4.602	21.513	1.00	72.43
40	ATOM	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
40	ATOM	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	ATOM	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
	ATOM	1791	C	LYS	529	42.813	-4.439	18.587	1.00	72.47
	ATOM	1792	0	LYS	529	43.990	-4.762	18.751	1.00	70.37
45	ATOM	1793	N	CYS	530	41.932	-5.191	17.930	1.00	74.48
43	ATOM	1794	CA	CYS	530	42.279	-6.474	17.325	1.00	76.67
	ATOM	1795	CB	CYS	530	41.004	-7.245	16.952	1.00	77.23
	MOTA	1796	SG	CYS	530	40.447	-8.491	18.146	1.00	79.38
	ATOM	1797		CYS	530	43.098	-6.220	16.065	1.00	78.08
50	ATOM	1798	0	CYS	530	43.241	-5.076	15.623	1.00	78.81
50	ATOM	1799	N	LYS	531	43.637	-7.289	15.487	1.00	78.22
	ATOM	1800	CA	LYS	531	44.424	-7.187	14.267	1.00	78.15
	ATOM	1801	CB	LYS	531	45.600	-8.182	14.305	1.00	78.33
	ATOM	1802	C	LYS	531	43.508	-7.467	13.067	1.00	77.93
5.5	ATOM	1803	0	LYS	531	42.549	-6.734	12.839	1.00	78.07
55	ATOM	1804	N	ASN	532	43.784	-8.539	12.328	1.00	77.80
	ATOM	1805	CA	ASN	532	42.984	-8.902	11.152	1.00	77.30
	ATOM	1806	CB	ASN	532	43.550	-10.166	10.521	1.00	77.55
	ATOM	1807	C	ASN	532	41.485	-9.082	11.423	1.00	77.34
60	ATOM	1808	0	ASN	532	40.904	-10.123	11.118	1.00	78.13
60	ATOM	1809	N	VAL	533	40.859	-8.055	11.988	1.00	76.13
	ATOM	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77

5	MOTA	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62
	ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
	MOTA	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
	MOTA	1814	С	VAL	533	38.685	-7.143	11.352	1.00	72.97
	ATOM	1815	0	VAL	533	39.024	-5.960	11.252	1.00	73.91
10	ATOM	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
	MOTA	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
	MOTA	1818	CB	LAV	534	35.619	-7.646	9.328	1.00	67.32
	ATOM	1819	С	LAV	534	36.463	-5.541	10.393	1.00	63.87
	ATOM	1820	0	VAL	534	35.895	-5.519	11.486	1.00	63.55
15	MOTA	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
	ATOM	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
	MOTA	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
	MOTA	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	MOTA	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
20	MOTA	1826	С	PRO	535	34.944	-2.902	10.571	1.00	52.90
	ATOM	1827	0	PRO	535	34.067	-3.461	9.908	1.00	52.01
	ATOM	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
	ATOM	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	ATOM	1830	CB	LEU	536	33.280	-0.796	13.128	1.00	44.35
25	ATOM	1831	CG	LEU	536	32.267	-0.911	14.273	1.00	43.48
	ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
	ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
	ATOM	1834	С	LEU	536	32.434	-1.433	10.871	1.00	43.58
	ATOM	1835	0	LEU	536	31.287	-1.862	10.734	1.00	42.14
30	ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
	MOTA	1837	CA	TYR	537	32.269	-0.066	8.866	1.00	43.34
	ATOM	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
	MOTA	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	ATOM	1840	CD1	TYR	537	32.190	0.964	5.687	1.00	48.46
35	ATOM	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
	MOTA	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99
	MOTA	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
	ATOM	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
	ATOM	1845	ОН	TYR	537	30.401	3.648	3.952	1.00	55.90
40	ATOM	1846	С	TYR	537	31.683	-1.199	8.032	1.00	43.15
	ATOM	1847	0	TYR	537	30.500	-1.191	7.696	1.00	41.54
	ATOM	1848	N	ASP	538	32.521	-2.175	7.702	1.00	44.67
	MOTA	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
	MOTA	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
45	ATOM	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
	MOTA	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	MOTA	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
	ATOM	1854	С	ASP	538	31.071	-4.195	7.587	1.00	43.48
	ATOM	1855	0	ASP	538	30.177	-4.738	6.940	1.00	43.95
50	ATOM	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
	MOTA	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	MOTA	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11
	ATOM	1860	CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
55	ATOM	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
	ATOM	1862	C .	LEU	539	28.891	-4.451	9.651	1.00	36.38
	ATOM	1863	ō	LEU	539	27.849	-5.070	9.436	1.00	35.74
	ATOM	1864	N	LEU	540	28.919	-3.146	9.894	1.00	35.50
	ATOM	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
60	ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
	ATOM	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28
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5	ATOM	1868	CD1	LEU	540	27.526	-1.299	12.645	1.00	38.55
	MOTA	1869	CD2	LEU	540	29.114		11.985	1.00	41.04
	ATOM	1870	C	LEU	540	27.060		8.510	1.00	35.50
	ATOM	1871	0	LEU.	540	25.846		8.371	1.00	33.21
	ATOM	1872	N	LEU	541	27.892		7.483	1.00	37.01
10	ATOM	1873	CA	LEU	541	27.418		6.101	1.00	38.51
	ATOM	1874	CB	LEU	541	28.591		5.145	1.00	39.67
	ATOM	1875	CG	LEU	541	28.301	-2.112	3.643	1.00	40.92
	ATOM	1876	CD1.		541	27.184		3.348	1.00	42.44
	ATOM	1877	CD2	LEU	541	29.572	-1.716	2.908	1.00	44.18
15	ATOM	1878	C	LEU	541	26.723		5.833	1.00	39.75
	ATOM	1879	0	LEU	541	25.616	-3.713	5.297	1.00	36.48
	ATOM	1880	N	GLU	542	27.366	-4.770	6.230	1.00	
	ATOM	1881	CA	GLU	542	26.790		6.037		40.88
	ATOM	1882	CB	GLU	542	27.719			1.00	41.89
20	ATOM	1883	CG	GLU	542	27.719		6.620	1.00	44.11
	ATOM	1884	CD	GLU	542	26.434		7.052	1.00	50.60
	ATOM	1885	OE1	GLU			-9.245	5.887	1.00	55.80
	ATOM	1886	OE1		542	25.570		6.130	1.00	58.81
	ATOM	1887	C	GLU	542	26.842	-8.996	4.728	1.00	57.19
25	ATOM			GLU	542	25.414	-6.195	6.691	1.00	41.58
23	ATOM	1888	0	GLU	542	24.472	-6.720	6.102	1.00	42.82
	ATOM	1889	N	MET	543	25.298	-5.686	7.915	1.00	40.09
		1890	CA	MET	543	24.036	-5.731	8.634	1.00	36.43
	ATOM	1891	CB	MET	543	24.270	-5.424	10.111	1.00	39.95
30	ATOM	1892	CG	MET	543	25.137	-6.459	10.808	1.00	41.95
30	ATOM	1893	SD	MET	543	24.918	-6.445	12.604	1.00	47.17
	ATOM	1894	CE	MET	543	25.324	-4.749	12.964	1.00	40.88
	ATOM	1895	C	MET	543	23.001	-4.769	8.072	1.00	35.02
	ATOM	1896	0	MET	543	21.808	-5.073	8.048	1.00	35.31
25	ATOM	1897	N	LEU	544	23.457	-3.605	7.629	1.00	32.90
35	ATOM	1898	CA	ΓΕÜ	544	22.559	-2.603	7.074	1.00	36.88
	ATOM	1899	CB	LEU	544	23.225	-1.226	7.111	1.00	34.51
	ATOM	1900	CG	LEU	544	23.268	-0.562	8.490	1.00	31.94
	ATOM	1901	CD1	LEU	544	24.284	0.564	8.478	1.00	32.27
40	ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
40	ATOM	1903	C	LEU	544	22.148	-2.941	5.640	1.00	38.94
	MOTA	1904	0	LEU	544	20.971	-2.842	5.294	1.00	39.52
	ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
•	ATOM	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	40.78
	ATOM	1907	CB	ASP	545	24.159	-3.780	2.620	1.00	37.75
45	ATOM	1908	CG	ASP	545	23.922	-3.937	1.120	1.00	35.19
	ATOM	1909	OD1	ASP	545	24.881	-4.265	0.380	1.00	33.48
	MOTA	1910	OD2	ASP	545	22.768	-3.734	0.691	1.00	31.33
	ATOM	1911	C	ASP	545	22.116	-5.015	3.349	1.00	42.87
	ATOM	1912	0	ASP	545	22.681	-6.030	2.929	1.00	44.32
50	MOTA	1913	N	ALA	546	20.853	-5.009	3.755	1.00	43.49
	ATOM	1914	CA	АĻĄ	546	20.069	-6.229	3.746	1.00	46.96
	ATOM	1915	CB	ALA	546	19.213	-6.305	5.006	1.00	47.82
	ATOM	1916	С	ALA	546	19.193	-6.362	2.508	1.00	49.55
	ATOM	1917	0	ALA	546	18.804	-5.368	1.883	1.00	48.75
55	ATOM	1918	N	HIS	547	18.895	-7.606	2.152	1.00	50.98
	ATOM	1919	CA	HIS	547	18.042	-7.884	1.006	1.00	53.77
	ATOM	1920	CB	HIS	547	18.431	-9.223	0.369	1.00	52.69
	ATOM	1921	CG	HIS	547	18.395	-10.382	1.317	1.00	55.05
	ATOM	1922	CD2	HIS	547		-10.362	2.242		
60	ATOM	1923	ND1	HIS	547				1.00	53.94
	ATOM	1924	CE1	HIS	547		-12.232	1.371	1.00	56.23
					J4 /	13.035	-14.232	2.286	1.00	55.36

5	ATOM	1925	NE2	UTC	C 4 7	32 024				
•	ATOM	1926			547	17.936				57.01
	ATOM	1927		HIS	547	16.603				55.69
	ATOM			HIS	547	16.362	-7.796	2.720	1.00	54.30
	ATOM	1928		ARG	548	15.653	-8.139	0.612	1.00	57.00
10		1929		ARG	548	14.245	-8.212	0.987	1.00	60.65
10	ATOM	1930		ARG	548	13.432	-7.171	0.208	1.00	62.69
	ATOM	1931		ARG	548	14.272	-6.222	-0.637		67.54
	ATOM	1932		ARG	548	13.448	-5.061	-1.171		71.92
	ATOM	1933		ARG	548	13.702	-3.826	-0.432		76.95
	ATOM	1934		ARG	548	14.864	-3.178	-0.429		79.04
15	ATOM	1935	NH1	ARG	548	15.891	-3.644	-1.128	1.00	80.66
	MOTA	1936	NH2	ARG	548	15.001	-2.063	0.278		
	ATOM	1937	C	ARG	548	13.695	-9.608			80.39
	ATOM	1938		ARG	548	12.500	-9.781	0.711	1.00	61.65
	ATOM	1939		LEU	549	14.576		0.466	1.00	62.05
20	ATOM	1940		LEU	549		-10.603	0.756	1.00	62.39
	ATOM	1941		LEU		14.188	-11.985	0.507	1.00	64.02
	ATOM	1942			549	15.433	-12.828	0.195	1.00	62.14
	ATOM	1943		LEU	549	16.461	-12.191	-0.753	1.00	60.76
	ATOM	1943		LEU	549	17.699	-13.074	-0.878	1.00	57.77
25	ATOM			LEU	549	15.823	-11.972	-2.108	1.00	58.38
23		1945		LEU	549	13.431	-12.574	1.702	1.00	66.65
	ATOM	1946	0	LEU	549	12.759	-13.600	1.577	1.00	67.15
	ATOM	1947		HIS	550	13.541	-11.920	2.856	1.00	67.72
	ATOM	1948	CA	HIS	550	12.858	-12.378	4.065	1.00	69.93
20	ATOM	1949	CB	HIS	550	13.753	-12.190	5.298	1.00	70.76
30	ATOM	1950	CG	HIS	550	14.977	-13.054	5.306	1.00	71.50
	ATOM	1951	CD2	HIS	550	15.539	-13.821	4.341	1.00	71.63
	ATOM	1952	ND1	HIS	550	15.793	-13.172	6.411	1.00	71.98
	ATOM	1953	CEI	HIS	550	16.805	-13.972	6.126	1.00	72.04
2.5	ATOM	1954	NE2	HIS	550	16.674	-14.379	4.876	1.00	71.39
35	ATOM	1955	C	HIS	550	11.556	-11.603	4.275	1.00	71.15
	ATOM	1956	0	HIS	550	10.940	-11.684	5.340	1.00	70.66
	MOTA	1957	N	ALA	551	11.143	-10.851	3.258	1.00	70.88
	ATOM	1958	CA	ALA	551	9.919	-10.057	3.338	1.00	
	ATOM	1959	CB	ALA	551	9.904	-9.014	2.221	1.00	73.58
40	MOTA	1960	С	ALA	551	8.658	-10.920	3.266		73.21
	ATOM	1961	0	ALA	551	7.684	-10.474		1.00	74.69
	ATOM	1962	OXT	ALA	551	8.651		2.621	1.00	76.12
	HETATM	1963	C10	OHT	600		1.481	3.852	1.00	73.79
	HETATM	1964		OHT	600	30.713			1.00	26.84
45	HETATM	1965	C8	OHT	600	31.366	-0.043	29.358	1.00	22.85
	HETATM	1966	C11	OHT	600		-0.385	28.037	1.00	25.56
	HETATM	1967		OHT	600	32.761	0.051	27.916	1.00	27.51
	HETATM	1968	C15	OHT	600	33.218	0.797	26.797	1.00	28.35
	HETATM	1969	C14			34.551	1.237	26.747	1.00	30.39
50	HETATM	1970	C13	OHT	600	35.443	0.923	27.792	1.00	30.23
	HETATM	1971		OHT	600	35.004	0.185	28.890	1.00	31.45
	HETATM	1972	C12	OHT	600	33.666	-0.241	28.955	1.00	27.93
	HETATM		C7	OHT	600	30.682	-1.089	27.077	1.00	24.41
	HETATM	1973	Cl	OHT	600	29.211	-1.258	27.052	1.00	24.26
55		1974	C2	OHT	600	28.644	-2.526	26.706	1.00	25.92
55	HETATM	1975	C3	OHT	600	27.254	-2.668	26.580	1.00	26.32
	HETATM	1976	C4	OHT	600	26.438	-1.553	26.813	1.00	29.02
	HETATM	1977	04	OHT	600	25.072	-1.605	26.716	1.00	28.42
	HETATM	1978	C5	OHT	600	26.980	-0.286	27.130	1.00	26.98
C C	HETATM	1979		OHT	600	28.362	-0.147	27.231	1.00	25.23
60	HETATM	1980	C17	OHT	600	31.370	-1.692	25.942	1.00	26.61
	HETATM	1981	C18	OHT	600	32.508	-2.498	26.151	1.00	26.77
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5	TTEM A COM	1982	C19	OHT	600	33.166	-3.052	25.072	1.00	27.50
3	HETATM	1983	C20	OHT	600	32.676	-2.794	23.786	1.00	27.50
	HETATM		020	OHI	600	33.206	-3.566	22.795	1.00	31.35
	HETATM	1984		OHT	600	33.009	-3.135	21.448	1.00	40.09
	HETATM	1985	C23	OHT	600	34.226	-3.490	20.575	1.00	44.80
10	HETATM	1986	C24	OHT	600	34.141	-4.901	20.203	1.00	49.00
10	HETATM	1987	N24		600	33.375	-5.040	18.933	1.00	51.64
	HETATM	1988	C25	OHT	600	35.495	-5.459	20.004	1.00	52.06
	HETATM	1989	C26	OHT	600	31.540	-2.005	23.558	1.00	27.19
	HETATM	1990	C21	OHT		30.892	-1.450	24.645	1.00	27.92
	HETATM	1991	C22	OHT	600		-12.010	23.057	1.00	27.20
15	HETATM	1992	01	нон	1	22.563	-0.070	25.819	1.00	25.77
	HETATM	1993	01	нон	2 3	25.183	19.202	23.149	1.00	42.52
	HETATM	1994	01	HOH		35.158	5.823	37.390	1.00	33.92
	HETATM	1995	01	нон	4	22.116	-9.922	18.914	1.00	30.18
	HETATM	1996	01	HOH	5	29.812	6.536	19.652	1.00	26.11
20	HETATM	1997	01	нон	6 7	13.362	4.463	20.376	1.00	29.40
	HETATM	1998	01	нон			-11.295	20.187	1.00	28.70
	HETATM	1999	01	нон	8	21.205	1.466	23.794	1.00	22.47
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WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof.

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

identifying a test compound that modulates coactivator binding to said nuclear receptor.

- The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.
- 3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.
 - 4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
- 5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
- 30 6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293. Ile302. Leu305. and Leu454.
 - 7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.
 - 8. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280. Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5

35

- residues Gln301. Ile302. Leu305. Lys306. helix 6 residue Cys309. and helix 12 residues Pro453. Leu454. Glu457. Val458 and Phe459.
 - 9. The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.
- 10
- 10. The method of claim 1, wherein said screening is in vitro.
- 11. The method of claim 10. wherein said screening is high throughput screening.
- 15 12. The method of claim 1, wherein said assay is a biological assay.
 - 13. The method of claim 1, wherein said test compound is from a library of compounds.
- 14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.
 - 15. The method of claim 14, wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.
- 25 16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.
 - 17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:
- providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;
 - modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and
- identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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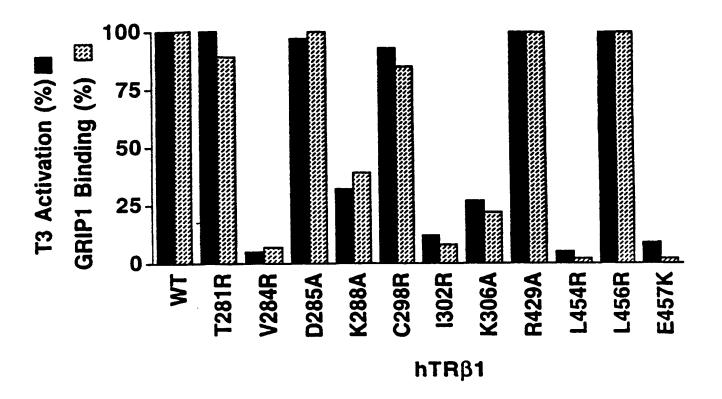
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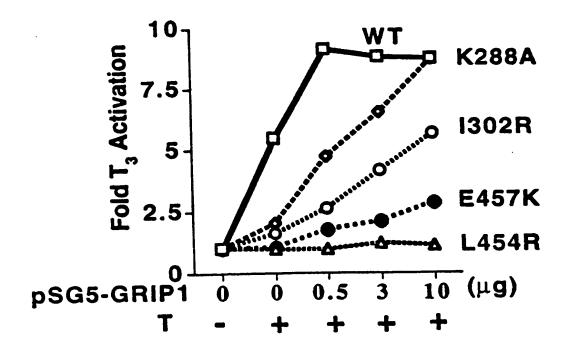
- 19. The machine readable storage medium of claim 18. wherein said nuclear receptor is a thyroid receptor.
- 20. The machine readable storage medium of claim 19, wherein said thyroid receptor is human.
 - 21. The machine readable storage medium of claim 20, wherein said molecule is peptide.
- 22. The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.
 - 23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
 - 24. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group

- 5 consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.
 - 25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.
 - 26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.
 - 27. The cocrystal of claim 26, wherein said thyroid receptor is human.
- 15 28. The cocrystal of claim 27, wherein said molecule is peptide.
 - 29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.
- 20 30. A compound identified according to the method of claim 1.

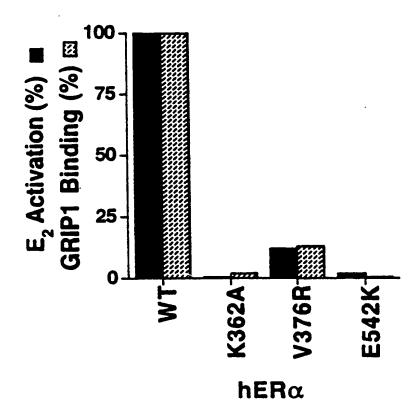
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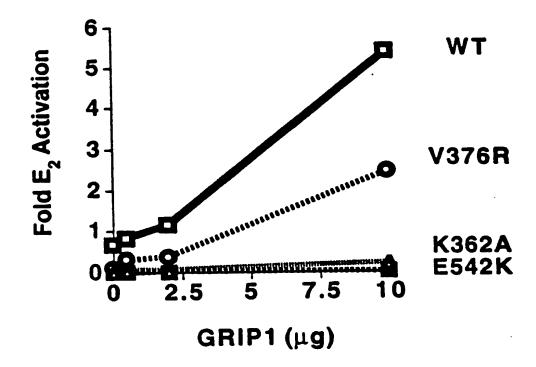


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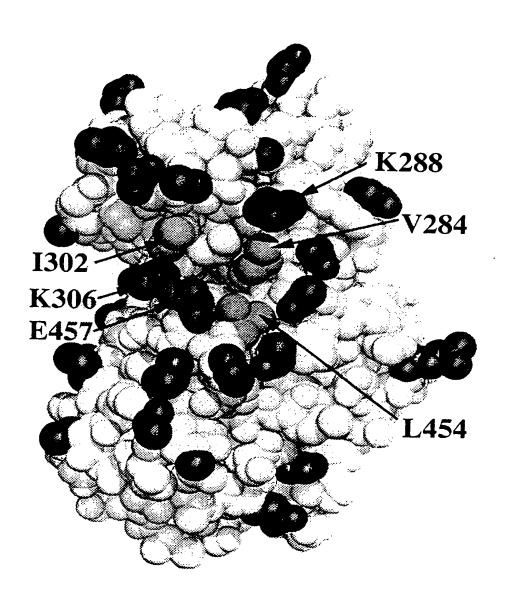


FIG. 5

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PAS

Overall Consensus (SEQ ID NO: 1)

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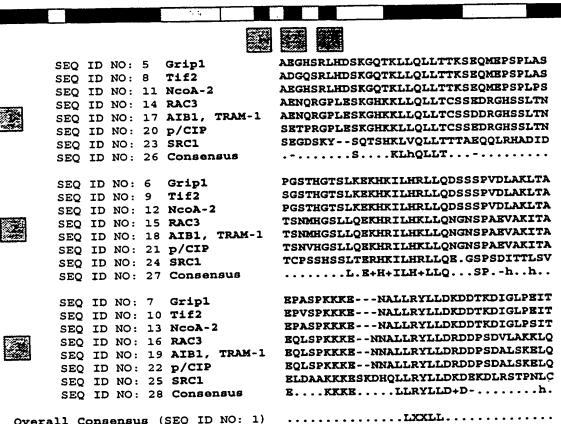
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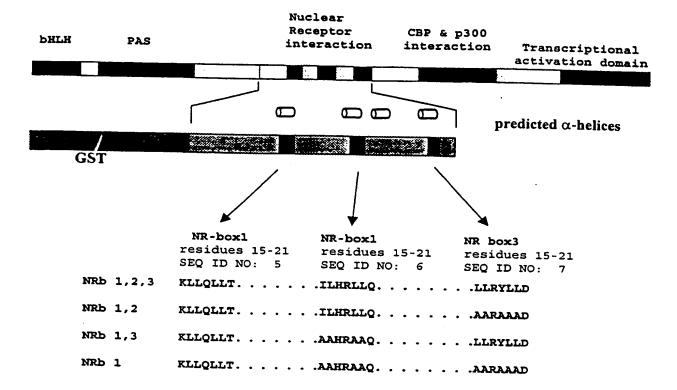
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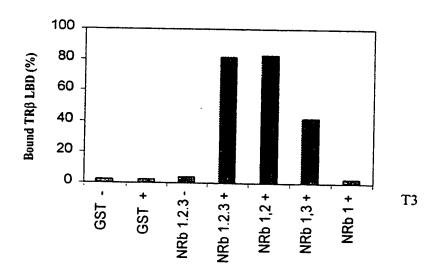
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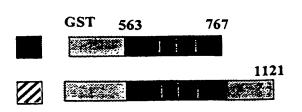
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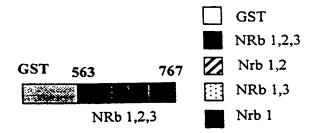


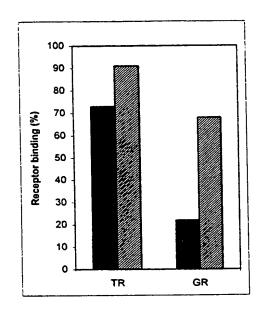


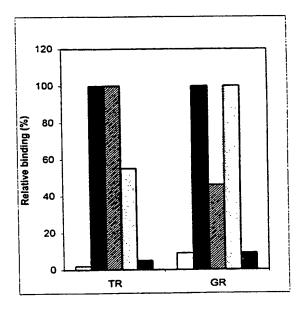


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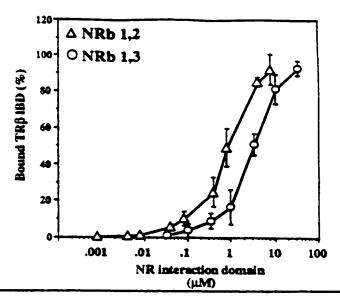


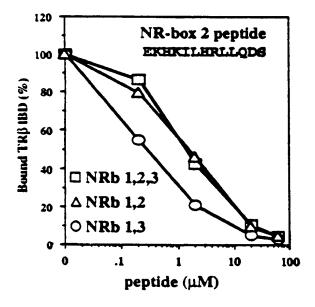


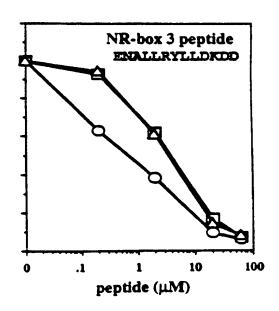




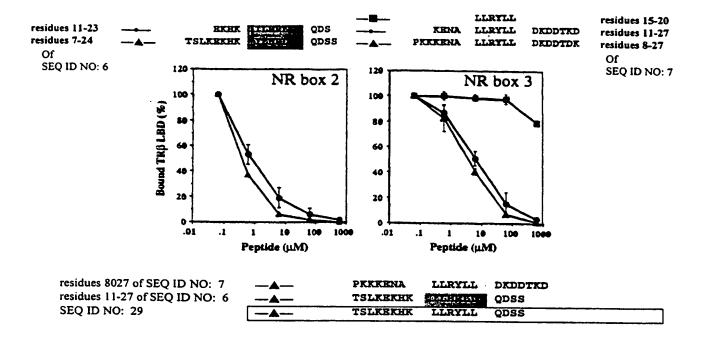
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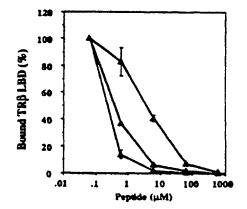


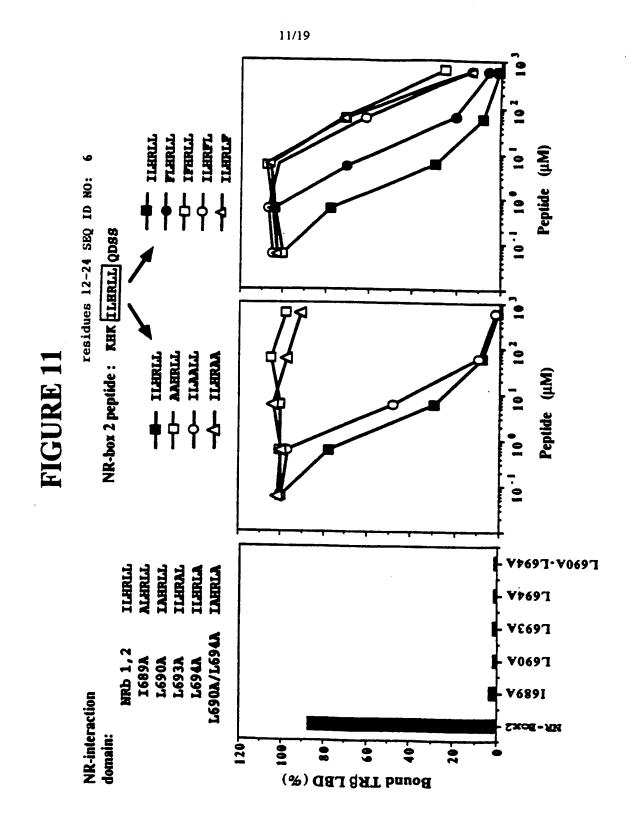




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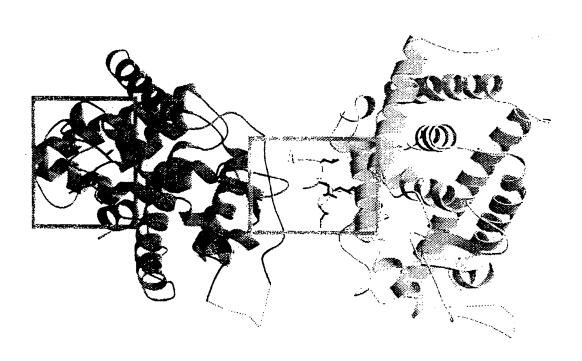


FIG. 12

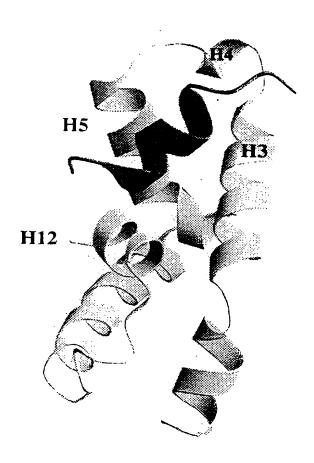


FIG. 13

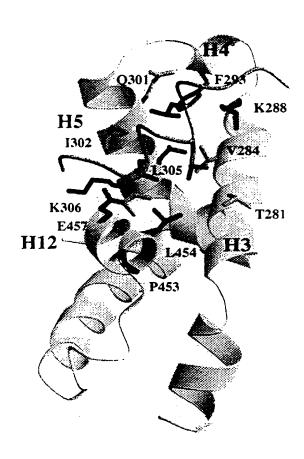


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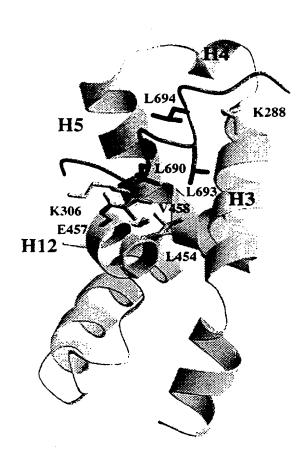


FIG. 15

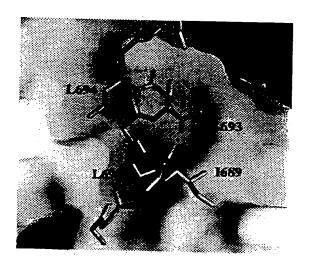


FIG. 16

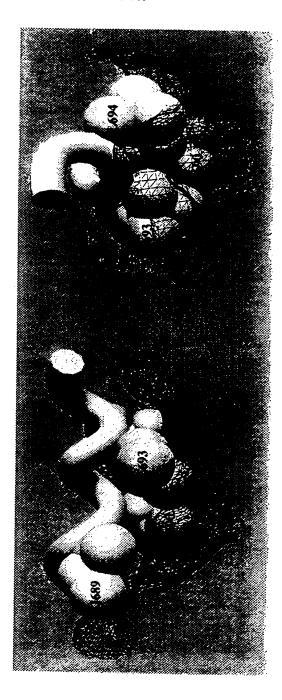


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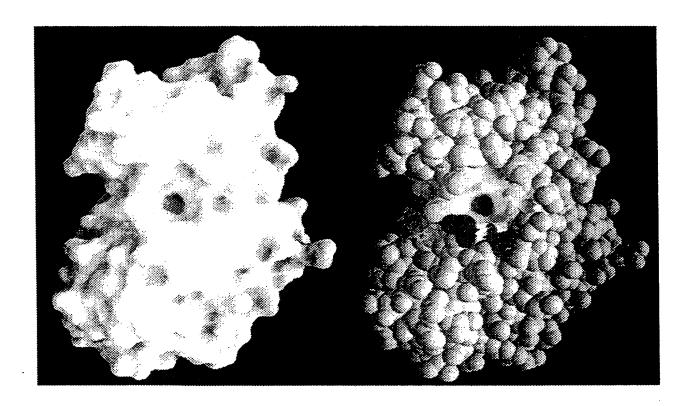
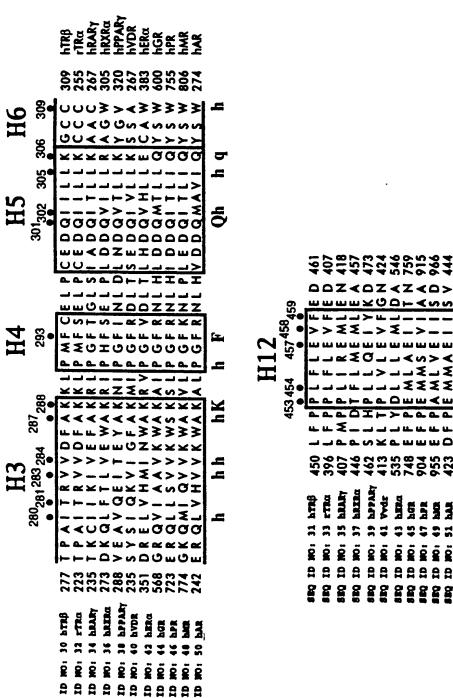


FIG. 18





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INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 7:	A3	(11) International Publication Number: WO 99/60014		
G01N 33/50		(43) International Publication Date: 25 November 1999 (25.11.99)		
(21) International Application Number: PCT/US (22) International Filing Date: 30 March 1999 (3000 El Camino Real, Five Palo Alto Square, Palo Alto,		
(30) Priority Data: 60/079,956 60/113,146 30 March 1998 (30.03.98) 16 December 1998 (16.12.9)	-	(81) Designated States: AU, CA, JP, KR, European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).		
 (71) Applicant: THE REGENTS OF THE UNIVERS CALIFORNIA [US/US]; 12th floor, 1111 Frankl Oakland, CA 94607-5200 (US). (72) Inventors: BAXTER, John, D.; 131 San Pablo Ave Francisco, CA 94127 (US). DARIMONT, Beatr Tenth Avenue, San Francisco, CA 94122 (US). Weijun; 105 Johnstone Drive, San Francisco, C (US). FLETTERICK, Robert; 15 Christopher Ave Francisco, CA 94131 (US). KUSHNER, Peter, 6th Avenue, San Francisco, CA 94122 (US). W Richard, L.; 1701 Waller Street, San Francisco, (US). WEST, Brian, L.; 142 Anderson Street, Scisco, CA 94110 (US). YAMAMOTO, Keith, R.; glass Street, San Francisco, CA 94114 (US). 	enue, Sice; 14 FEN CA 941 enue, S J.; 13 /AGNE CA 941 San Fra	(88) Date of publication of the international search report: 18 May 2000 (18.05.00) 18 May 2000 (18.05.00) 18 R, 17 n-		

(54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(57) Abstract

The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

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INTERNATIONAL SEARCH REPORT

Inconational application No.
PCT/US99/06899

A. CLASSIFICATION OF SUBJECT MATTER IPC(7) :G01N 33/50				
US CL :435/7.1				
According to International Patent Classification (IPC) or to both national classification and IPC				
B. FIELDS SEARCHED				
Minimum documentation searched (classification system followed	by classification symbols)			
U.S. : 435/7.1				
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched				
Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Extra Sheet.				
C. DOCUMENTS CONSIDERED TO BE RELEVANT				
Category* Citation of document, with indication, where ap	Citation of document, with indication, where appropriate, of the relevant passages			
X WAGNER et al. A structural role		1		
hormone receptor. Nature. 14 Decer A 690-697, especially page 690 and figure		2-30		
oso-osi, especially page oso and light	ic I and 2 and I able I.	2-30		
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01 DECEMBER 1999 2 9 FEB 2000				
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INTERNATIONAL SEARCH REPORT

International application No. PCT/US99/06899

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)					
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:					
1. Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:					
2. Claims Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:					
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).					
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)					
This International Searching Authority found multiple inventions in this international application, as follows:					
Please See Extra Sheet.					
As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.					
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.					
As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:					
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:					
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No protest accompanied the payment of additional search fees.					

Form PCZ/ISA/210 (continuation of first sheet(1))(July 1992)*

CORRECTED VERSION

(19) World Intellectual Property Organization International Bureau





(43) International Publication Date 25 November 1999 (25.11.1999)

PCT

(10) International Publication Number WO 99/060014 A3

(51) International Patent Classification7: G01N 33/50

PCT/US99/06899 (21) International Application Number:

(22) International Filing Date: 30 March 1999 (30.03.1999)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

60/079,956 60/113,146 30 March 1998 (30.03.1998) US

16 December 1998 (16.12.1998)

- (71) Applicant: THE REGENTS OF THE UNIVERSITY OF CALIFORNIA [US/US]; 12th floor, 1111 Franklin Street, Oakland, CA 94607-5200 (US).
- (72) Inventors: BAXTER, John, D.; 131 San Pablo Avenue, San Francisco, CA 94127 (US). DARIMONT, Beatrice; 1441 Tenth Avenue, San Francisco, CA 94122 (US). FENG, Weijun; 105 Johnstone Drive, San Francisco, CA 94131 (US). FLETTERICK, Robert; 15 Christopher Avenue, San Francisco, CA 94131 (US). KUSHNER, Peter, J.; 1362 6th Avenue, San Francisco, CA 94122 (US). WAGNER, Richard, L.; 1701 Waller Street, San Francisco, CA 94117 (US). WEST, Brian, L.; 142 Anderson Street, San Francisco, CA 94110 (US). YAMAMOTO,

Keith, R.; 332 Douglass Street, San Francisco, CA 94114 (US).

- (74) Agents: HUNTER, Tom et al.; Law Offices of Jonathan Alan Quine P.O. Box 458, Alameda, CA 94501 (US).
- (81) Designated States (national): AU, CA, JP, KR.
- (84) Designated States (regional): European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).

Published:

— with international search report

- (88) Date of publication of the international search report: 18 May 2000
- (48) Date of publication of this corrected version:

29 August 2002

(15) Information about Correction:

see PCT Gazette No. 35/2002 of 29 August 2002, Section п

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(57) Abstract: The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to these sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.

WO 99/060014 PCT/US99/06899

METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

ACKNOWLEDGEMENTS

This invention was supported in part by grants from the National Institutes of Health: Grant Nos. DK 51083, DK 51281, and P41-RR01081 and from the Army of the United States: Grant No. AIBS#562. The U.S. Government may have rights in this invention.

INTRODUCTION

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Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

Although overall sequence conservation between nuclear receptors varies between different families of receptors, sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to modulate transcription of DNA, although they may have transcription-independent actions. Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear receptors on transcription. For example, nuclear receptors can stimulate transcription in response to hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al., Curr. Opin. Cell Biol. (1997) 9:222-32); and Horwitz et al., Mol. Endocrinol. (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain, called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253; VDR: Jurutka et al., J. *Biol. Chem.* (1997) 227:14592-14599, Masayama et al., *Mol. Endocrinol.* (1997) 11:1507-1517; ER and RAR: Henttu et al., *Mol. Cell Biol.* (1997) 17:1832-1839). While these studies support the physiological relevance of the observed interaction, the structural and functional nature of the site to which coactivators bind has not been defined.

The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism, hypercholesterolemia, obesity and other conditions. However, limited treatments are available and current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors are desired for drug development, the structural and functional basis of such sites, including the coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator proteins. This would provide a major new target for iterative drug design, synthesis, and selection. It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target the coactivator binding site of nuclear receptors and administer them to organisms to modulate physiological processes regulated by nuclear receptors.

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5 Relevant Literature

Wagner et al., (Nature (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., supra; O'Donnell et al., Mol. Endocrinol. (1991) 5:94-99; Whitfield et al., Mol. Endocrinol. (1995) 9:1166-79; Saatcioglu et al., Mol. Cell Biol. (1997) 17:4687-95; Collingwood et al., supra; Kamei et al., Cell (1996) 85:403-14). Hong et al. (Proc. Natl. Acad. Sci. USA (1996) 93(10):498-49452) and Hong et al. (Mol. Cell. Biol. (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (Nature (1997) 387:677-84), Le Douarin et al., (EMBO J (1996) 15:6701-6715) and Heery et al. (Nature (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

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SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by

5 binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator

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binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors. The unique features involved in receptor-selective coactivator binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

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BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the specific effects of mutations on hTRβ1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T₃ dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant. GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

Figure 2 shows that overexpression of full-length GRIP1 rescues loss of transcriptional activation by hTRβ1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in Figure 1. The WT or different representative hTRβ1 mutants are indicated.

Figure 3 shows specific hERα surface mutants cause loss of transcriptional activation in HeLa cells in parallel with their loss of *in vitro* GRIP1 binding. The fold E₂ activation, expressed as the percentage of WT, and the phosphorimager quantitation of *in vitro* binding of [³⁵S]-labeled hERα WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

Figure 4 shows a plot of the fold E₂ activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for Figure 3. The WT or different hERα mutants are indicated. The data represent the averages of three independent experiments, with standard deviations less than 10%.

Figure 5 shows a CPK model of the TRα-LBD, indicating the LBD surface locations of mutations made in the full-length hTRβ1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1a binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues, respectively. The main chain structures of the TRα- and TRβ-LBDs are the same (data not shown).

Figure 6 shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

Figure 7 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TRβ LBD. Single letter designations are used for the amino acids.

Figure 8 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

Figure 9 shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

Figure 10 shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of NR-box-TR β LBD interactions.

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Figure 11 shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TRβ LBD.

Figure 12 shows the contents of the asymmetric unit of the crystallized hTR\$ LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in both bound peptides.

Figure 13 shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTRß LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of α-helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTRß LBD, and the neighboring monomer, are omitted for clarity.

Figure 14 shows interface between the GRIP1 NR-box 2 peptide and the hTRß LBD. Side chains of residues of the hTRß LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID NO: 2) ILxxLL motif shown explicitly.

Figure 15 shows residues in the hTRB LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTRB LBD.

Figure 16 shows molecular surface of the hTR LBD. The side chains of the leucines resides fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

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Figure 17 shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucince residues fit into pockets of the coactivator binding site of the hTRB LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

Figure 18 shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft 15 and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

Figure 19 shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

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DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR

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residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus,

for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

Compounds of particular interest fit spacially and preferentially into the coactivator binding By "fits spacially and preferentially" is intended that a compound possesses a threedimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single

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gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α, β) or three (RAR, RXR, and PPAR: α, β, γ) genes or have alternate RNA splicing.

The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in Figure 19). As described in the Examples, the cocrystal of the hTRB LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide. Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO: 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

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For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be used to predict how a small molecule of interest can interact with the nuclear receptor coactivator binding site. Fragment-based docking also can be used in building molecules *de novo* inside the coactivator binding site, by placing chemical fragments that complement the site to optimize intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR), using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and

5 molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, J. Med. Chem. (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., Proteins: Structure, Function and Genetics, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., Proteins: Structure, Function and Genetics (1990) 8:195-202; available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, J. Mol. Biol. (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

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Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA; reviewed in Martin, *J. Med. Chem.* (1992) 35:2145-2154); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., J. Med. Chem. (1990) 33:883-894); Navia et al., Curr. Opin. Struct. Biol. (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, for example, Farmer, "Drug Design," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, Structure, (1994) 2:577-587); and Kuntz et al., Science, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity, such as a biologically based assay. Screening can be *in vitro* and/or *in vivo*. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening

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preferably centers on activity-based response models, binding assays (which measure how well a 5 compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

As an example, in vitro binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein and in Shibata et al. (Recent Prog. Horm. Res. 52:141-164 (1997)); Tagami et al. (Mol. Cell Biol. (1997) 17(5):2642-2648); Zhu et al. (J. Biol. Chem. (1997) 272(14):9048-9054); Lin et al. (Mol. Cell Biol. (1997) 17(10):6131-6138); Kakizawa et al. (J. Biol. Chem. (1997) 272(38):23799-23804); and Chang et al. (Proc. Natl. Acad. Sci. USA (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., MCB supra; and 25 Hong et al., PNAS supra) and/or SRC-1 (Spencer et al., Nature (1997) 389:194-198; Onate et al., Science (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

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Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples, TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T₃.

Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

After the three dimensional structure of the cocrystal is determined, the structural information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful for solving the structure of those other crystal forms of nuclear receptors. They may also be used to

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solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in Appendix 1. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interative drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors

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that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR-α, human RAR-γ, human RXR-α, human PPAR-α, human PPAR-β, human PPAR-γ, human VDR, human ER (as described in Seielstad et al., Molecular Endocrinol., (1995) 9:647-658, incorporated herein by reference), human GR, human PR, human MR, and human AR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2. A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong et al. (PNAS <u>supra</u>; and MCB <u>supra</u>), for GRIP1 expression, which reference is herein incorporated by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR-α or Glu 202 to Asp 461 of the human TR-β.

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

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To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA*, (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute

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components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the handing drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., <u>supra</u>. The structure is refined following standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

EXAMPLES

Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators

A. Human TRβ LBD

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Human TRß LBD (His6-E202-D461) was expressed and purified as described (Shiau et al., Gene (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28) in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for 24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl, 10% glycerol, 25mM ß-merceptoethanol and 0.1mM PMSF as described above. The lysate was cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an imidazole gradient (12 - 300 mM). TRB LBD containing fractions were loaded in 0.6M ammonium sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium sulfate gradient [0.6 - 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TRB LBD were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T₃ (Sigma). The hydrophobic interaction run was repeated with liganded receptor under the same conditions. Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed to 20mM Hepes pH7.0, 3mM DTT and 0.1 µM T₃ using NAP columns (Pharmacia). For crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10 concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter bacterial culture.

B. Human TR mutants

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded oligonucleotides which encode the mutant sequence and which have ends allowing them to be ligated as a cassette using pairs of the NsiI, PstI, SstI, AlwNI, ApoI, PflMI, BstXI, BseRI, BsmFI, PvuII, NspI, SmaI, PmII, BglII and BsmI restriction sites of the hTRβ1 cDNA sequence, or the 3' plasmid polylinker SalI, or BamHI restriction sites. The hTRβ1 sequences thus mutated were subcloned into the pCMX vector encoding the full-length 461 amino acid hTRβ1 sequence. Some of the mutations of the hTRβ1 in the CMX vector and all three mutations of the hERα in the pSG5-ER-HEGO vector (Tora et al., EMBO (1989) 8:1981) were created using Quick Change Site-

5 Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

C. Human ERa LBD

The human ERα-LBD 297-554 was overexpressed as described previously (Seielstad, et al., supra) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained the sequence Met-Asp-Pro fused to residues 297 to 554 of the hERα (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., Proc. Natl. Acad. Sci. USA (1980) 77:5115-5119; Landel, et al., Mol. Endocrinol. (1994) 8:1407-1419; Landel, et al., J. Steroid Biochem. Molec. Biol. (1997) 63:59-73).

To carboxymethylate the solvent-accessible cysteines, the bound hERα-LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., Steroids (1996) 61:367-373). Protein was eluted with 3 x 10-5 M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hERα-LBD was typically close to 100% (Seielstad, et al., Biochemistry (1995) 34:12605-12615). The affinity-purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hERα-LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass spectrometry.

D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ERα LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ³⁵S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

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³⁵S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hERα LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376; L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

E. Human ER LBD-GST Fusion Protein

A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hERα was constructed by subcloning the EcoRI fragment from pSG5 ERα-LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

F. Radiolabeled full-length receptors and coactivator proteins

Wild-type (WT) or mutant pCMV-hTRβ1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [35 S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTRβ1 (full-length, WT or mutants, WT provided by. C. Costa), and the GST-hRXRα (full-length

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5 provided by. C. Costa), fusion proteins were produced in E. coli strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

G. Coactivator GRIP1 563-767 His6 GST fusion protein

GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1 563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I-Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX 10 GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 15 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freezethawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered 20 (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion 25 fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliquts and stored at -70°C.

30 H. Coactivator GRIP1 563-767 His6

GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived fron pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl

pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

Example 2: Peptide synthesis

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Coactivator peptides were obtained using standard techniques. All peptides were HPLC purified and analyzed by mass spectroscopy. Peptide concentrations were either determined spectroscopically using the tyrosine signal ($A_{276} = 1450 \text{ M-1cm-1}$) or by amino acid analysis following standard techniques.

Example 3: Binding assays with nuclear receptors and coactivators

A. GST-GRIP Pull-down Assays and Peptide Competition Assays

Binding experiments were performed by mixing glutathione beads containing 10 μ g of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2 μ l of the [35 S]-labeled wild-type or mutant hTR β 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150 μ l of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM MgCl₂, 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the presence or absence of 1 μ M T₃. Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

For *in vitro* binding studies GR, TR and their derivatives were translated in the presence of [35S]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were performed in the presence and absence of 10µM dexamethasone or 1µM RU486 for GR and 10µM triiodothyronine for TR. Expression was quantified by phosphoimager analysis (BAS2000, Fuji). For all binding assays 50µl of a 20% bead suspension containing either 1.6 or 4.0 µM bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2µl or 1.4µl *in vitro* transcribed and translated TR or GR, respectively. Binding was performed in the binding buffer described above supplemented with 20 µg/ml BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of

receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200μl binding buffer + BSA at 4°C before elution of the bound proteins in 20μl SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was determined by phosphoimager analysis.

B. GST-hTRβ1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [³⁵S]-labeled full-length GRIP1, [³⁵S]-labeled full-length SRC-1a, and [³⁵S]-labeled full-length hRXRα, to GST-hTRβ1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and E457K all bound to hRXRα with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [³⁵S]-Met-labeled full-length hTRβ1 WT and mutants (data not shown).

20 C. GST-hERα LBD Pull-down Assays

The wild-type and mutant GST-hERα LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hERα (H222). Cleared extracts containing the GST- hERα LBDs were incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μM of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μl glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. ³⁵S-labeled GRIP1 was synthesized by *in vitro* transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hERα LBDs were incubated for 2.5 hours with 2.5 μl aliquots of crude translation reaction mixture diluted in 300 μl of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40,

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5 proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound ³⁵S-GRIP1 was quantitated by fluorography following SDS-PAGE.

D. Electrophoretic Mobility Shift Assays

GRIP1, a mouse p160 coactivator, recognizes the ER α LBD in a ligand-dependent manner. The binding of agonists to the ER α LBD promotes recruitment of GRIP1, whereas binding of antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ER α strongly prefers NR-box 2 (Ding, et al., *Mol. Endocrinol.* (1998) 12:302-13).

An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ERa LBD in the presence of either DES or OHT. Eight microgram samples of purified hERa-LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10 µl of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

In the presence of the NR-box 2 peptide, the migration of the DES-hER α -LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hER α -LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

Example: 4 Transfection assays with TR and hERa

HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5 μg of the reporter p(DR-4)₂ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results (data not shown). Also, 2 μg of the hTRβ1 expression vector, pCMX-TR (WT or mutant), and 0.5 μg transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the β-galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s),

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or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., <u>supra</u>), and GC cells expressing TR (Norman et al., *J. Biol. Chem.* (1989) 264:12063-12073).

For hER α assays, 5 µg of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, et al., Mol Cell Biol. (1995) 15:1554), 0.5 µg expression vector encoding full-length hER α , pSG5-er HEGO (WT or mutants), and 2 µg of pj3lacz, were used. For the experiments of Figures 2 and 4, 0.5 µg of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were treated with or without 1 µM T₃ or E₂, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the β -galactosidase activities were also assayed to correct for differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

Example 5: Hormone binding assays for wild-type and mutant TRs

The T_3 binding affinity constants (Kd) for *in vitro* -translated WT and mutant TRs were measured using [$^{125}\Pi$] 3,5,3' triiodo-L-thyronine ([$^{125}\Pi$ T₃) in gel filtration binding assays as described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the Kd and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81 ± 12 pM. The relative affinity was determined by dividing the WT Kd by each mutant Kd. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T₃) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent

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5 (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (Figure 1). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (Figure 1). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators recognize the same TR surface residues.

Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T₃ increased reporter gene activity 5-fold in cells expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in Figure 1. By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T₃ which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of GRIP1 binding and activation (Figure 2). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

Example 8: Effect of TR mutations on other receptor functions

The effects of the mutations on other receptor functions also were examined. All of the mutants bound radiolabeled thyroid hormone (Kd values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., *supra*; Lee et al., *Mol. Endocrinol.* (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T3-dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., *supra*), suggesting that the CBS residues do not participate in TR actions mediated through these proteins. These data

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indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

Example 9: Coactivator binding site in ER

Three separate mutations (K362A, V376R, and E542K) were created in human estrogen receptor-α (hERα) which align to three of the effective positions in hTRβ1 (K288A, I302R, and E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which responds to the ER amino-terminal activation function (Berry et al., EMBO J (1990) 9:2811-2818) (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

Example 10: Coactivator NR-box binding affinity for TR

To study the interaction between nuclear receptors and GRIP1 in vitro, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTRß LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0 μ M) over NR-box 3 (EC50 = 4.0 μ M) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR.

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Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

Example 11: Coactivator NR-box binding affinity for GR

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial antagonist RU486. These results are in agreement with *in vivo* 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

Example 12: Coactivator peptide binding affinity for TR

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTR3 LBD were performed using coactivator peptides containing different NR- boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLLQDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (Figure 9). Consistent with the interaction of hTR LBDB with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of GRIP1 with hTRB LBD only at very high concentrations (EC50 = 130 μ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTRB LBD for NR-box 2 (EC50 (NR-box 2) = 1.5 μ M, EC50 (NR-box 3) = 4 μ M). The apparent affinities (EC50) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the sequence and independent of the structural context of the NR-boxes.

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Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes, TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

Example 13: Binding affinity of TR for extended coactivator peptides

Sequence identity between all three central NR-boxes of the p160 coactivator family is limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (Figure 6). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTR\$ LBD were compared (Figure 10).

A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

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5 Example 14: Binding affinity of TR and GR for mutant coactivator

A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRLL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (Figure 11). Surprisingly, replacement of any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTR\$ LBD, it appears that their contribution to the affinity of NR-box 2 for hTR\$ LBD is cooperative rather than additive.

Similar results were obtained by competing the interaction of hTR3 LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (Figure 11). Whereas the peptides containing the IL or LL replacement failed to interact with the hTR3 LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (Figure 11). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTRB LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767) with hTR\$\text{LBD}\$.

B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTRß LBD:NR-box 2 interaction surface, whereas the non conserved

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isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTR\$\beta\$ LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-KHKILHRLLQDSS-698 is highly complementary to the corresponding binding site in the hTR\$\beta\$ LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., Nat Struct Biol. (1996) 3:87-94; Wagner et al., supra; Renaud et al., Nature (1995) 378:681-689; Bourguet et al., Nature (1995) 375:377-382; and Brzozowski et al., Nature (1997) 389:753-758).

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic alphahelices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL) differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a

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5 GRIP1 mutant lacking NR-box 3, binds GR in vivo (Ding et al., <u>supra</u>). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).

These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

C. TR affinity for residues adjacent to ILxxLL motif

Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (Figure 11). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

Example 15: Crystallization and Structure Determination of NR LBD Complexes

A. Crystallization of hTRB LBD with T₃ and GRIP1 NR-box 2 Peptide

Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the 30 hTR\$ LBD. The complex of the hTR\$ LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTR\$ LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding

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of prepared drops with microcrystals of the hTRB LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTRB LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTRB LBD determined previously (Wagner et al., supra), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTRß LBD, residues K211-P254 and G261-D461 of monomer 2 of the hTRB LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-10 KILHRLLQDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLLQD-696 (Appendix 1).

Briefly, the complex between the hTRß LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal) volumes of a solution of 9mg/ml hTRß LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTRB LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10-3 to 10-5 dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTRB LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

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Table 1

Data collection, phasing, and refinement statistics

			Da	ta collection	1	
Data set		lution Å)	Reflec	ctions	Coverage (%)	R _{sym}
Native	3	3.6 measure 35565		unique 8490	96.3	0.007
			Ro	tation searc	h	
Search model		Eule	er angles (°)		Correlation	on coefficient
		Θ_1	Θ_2	Θ ₃	Highest peak	Highest false pea
hTR β LBD	M1	60.12	80.68	241.90	16.3	
	M2	9.93	87.70	180.6	15.9	14.2
<u></u>			Tra	nslation sea	rch	
			Fractional co	ordinates	Tran	slation function
		x	У	Z		Highest false peak (c
	MI	0.522	0.42	8 0.250	19.52	10.02
	M2	0.200	0.93	0.119	26.11	5.77
				Refinement		
	Re	esolution (Å)	R	eflection	R	R _{free}
F > 2(25 - 3.7		7614	0.2990	0.3219
All data	 	25 - 3.7		7851	0.3010	0.317

 $R_{\text{sym}} = \Sigma_h \Sigma_i \mid I_{h,i} \hat{\mathbf{u}} \left(I_h(\mid / \Sigma I_h \text{ for the intensity } (I) \text{ of } i \text{ observations of reflection } h.$ Correlation coefficient = $\Sigma_h Eo^2 Ec^2 - Eo^2 Ec^2 / \left[\Sigma_h \left(Eo_2 - Eo^2 \right)^2 \Sigma_h \left(Ec^2 - Ec^2 \right)^2 \right]^{1/2}$ Translation function $(t_a, t_b, \ldots) = \Sigma_h \left(|Eo_{(h)}|^2 - \Sigma_h < |Eo_{(h)}|^2 > \right) \left(Ec_{(h, t_a, t_b, \ldots)} \right)^2 - < |Ec_{(h)}|^2 \right)$ where E_o represents the normalized observed structure factor amplitudes, and E_c represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation

(ta, tb) of the NCS monomers, divided by the rms value of the translation

function density.

R factor = $\Sigma |F_{\text{obs}} - F_{\text{calc}}| / \Sigma |F_{\text{obs}}|$. R_{free} is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

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B. Crystallization of hERα LBD with DES and GRIP1 NR-box 2 Peptide

Crystals of a DES-hERa LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hERa LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two μL samples of this solution were mixed with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μ L of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2₁ with cell dimensions a=54.09, b=82.22, c=58.04 and β=111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200 μm x 40 μm x 40 μm crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μM peptide and frozen in an N2 stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., Methods Enzymol. (1997) 276:307-326) using the default -3 σ cutoff.

C. Crystallization of hERa LBD with OHT

Crystals of the hER α LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μ L) of a solution containing 3.9 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6₅22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit consists of a single hER α LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μ m x 250 μ m x 40 μ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N₂ suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a

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5 wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., *supra*) using the default -3σ cutoff.

Example 16: Structure determination and refinement of NR LBD complexes

A. Structure of hTRB LBD with T₃ and GRIP1 NR-box 2 Peptide

Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In Macromolecular Crystallography, Part A (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in AMORE from a model of hTRB LBD with the ligand, T3, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTRB LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTRB LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and conventional difference Fourier maps for the iodine atoms of the T3 ligand confirmed the correctness of the solution. The iodine atoms for both T3 ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTRß LBD. The electron density could be modeled as a short α-helix, and the observed side chain density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTRB LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLLODSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTRB LBD:GRP1 site 2 peptide complex are attached as Appendix 1.

B. Structure of hERa LBD with DES and GRIP1 NR-box 2 Peptide

Initial efforts to determine the structure of the DES-hER α LBD-NR box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4

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suite: programs for protein crystallography", Acta Crystallogr. (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RARy LBD (Renaud, et al., supra) as the search probe (R=58.2%, CC=35.6% after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 Å between this model and the final model based on Ca positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., Bull. Soc. Chim. Belg. (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., Acta Crystallogr. (1997) D53:240-255) (using tight NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 Am. Cryst. Assoc. Mtg. Abstr. (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of weights.

However, although the DES-hERa LBD-NR complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hERa LBD-NR-box 2 peptide complex became available when the R_{free} of the OHT-hER α LBD model was ~31%. Both monomers in the asymmetric unit of the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hER α LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximumlikelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 Å (with no o cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hER α

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5 LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% (R_{free}=25.0%) using data to 2.03 Å resolution.

Ile 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The γ-carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 377, the γ-carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ERα LBD (Eng, et al., *Mol. Cell. Biol.* (1997) 17:4644-4653); Lazennec, et al., *Mol. Endocrinol.* (1997) 11:1375-86; White, et al., *EMBO J.* (1997) 16:1427-35). Atomic coordinates of DES-LBD-peptide complex are attached as Appendix 2.

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Summary of Crystal		istics
	Liga	nd
Data Collection	<u>DES</u>	<u>OHT</u>
Space group	P2 ₁	P6 ₅ 22
Resolution	2.03	1.90
Observations	104189	269253
Unique	30265	23064
Completeness (%)	98.4	99.1
R _{sym} (%) ^a	7.8	7.0
Average I/oI	9.8	16.1
Refinement		
Number of non-hydrogen atoms	4180	2070
R_{cryst} (%) $^b/R_{free}$ (%)	19.9/25.0	23.0/26.1
Bond r.m.s. deviation (Å)	0.006	0.006
Angle r.m.s. deviation (°)	1.05	1.05
Average B factor (Ų)	34.0	40.4
a $R_{sym} = \sum_i I_i - \langle I_i \rangle / \sum_i$	$\sum_{i} I_{i}$ where $\langle I_{i} \rangle$	is the average intensity
over symmetry equiv	valents	
$^{b} \qquad R_{cryst} = \sum F_{o} - F_{c} /$	$\sum F_{o} $	
	Space group Resolution Observations Unique Completeness (%) $R_{sym}(\%)^a$ Average I/ σ I Refinement Number of non-hydrogen atoms R_{cryst} (%) $^b/R_{free}$ (%) Bond r.m.s. deviation (Å) Angle r.m.s. deviation (°) Average B factor (Å ²) a $R_{sym} = \sum_i I_i - \langle I_i \rangle /I_i$ over symmetry equiv	Space group P2 ₁ Resolution 2.03 Observations 104189 Unique 30265 Completeness (%) 98.4 $R_{sym}(\%)^a$ 7.8 Average I/ σ I 9.8 $\frac{Refinement}{R_{cryst}} (\%)^b/R_{free} (\%)$ 19.9/25.0 Bond r.m.s. deviation (Å) 0.006 Angle r.m.s. deviation (°) 1.05 Average B factor (Å ²) 34.0 $R_{sym} = \sum_i I_{i^-} < I_{i^-} / \sum_i I_i \text{ where } < I_{i^-} < $

C. Structure of hERa LBD-OHT complex

The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERα LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6₁22 and P6₅22. A translation search in P6₅22 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hERα LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR

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5 (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., *Proc. Natl. Acad. Sci. USA* (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the R_{free} set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no σ cutoff) were included. The final model consisted of residues 306-551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hERα LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% (R_{free}=26.2%). Atomic coordinates of OHT-hERα LBD complex are attached as Appendix 3.

15 Example 17: Structural analysis of hTRB LBD:GRIP 1 NR-box 2 peptide complex

A. Structure of cocrystal complex (contents of asu)

The asymetric unit (asu) of the crystal contains two monomers of the hTRß LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (Figure 12). The structure of the hTRß LBD, which closely resembles that of the rTRα LBD (Wagner et al., supra), consists of twelve alpha-helices and two β-strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTRß LBD and the rTRα LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic α-helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

The relation of the two monomers of the hTRß LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., <u>supra</u>; Brzozowski et al., <u>supra</u>). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the alpha-helix of the cocrystal peptide contacts monomer 1 of the hTRß LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

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The common interface between both cocrystal peptides and the hTR\$ LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTR\$ LBD, while the hydrophilic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

B. Structure of the GRIP1 NR-box 2 peptide

The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLLQDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., Science (1996) 274:948-953), VP16:TAF31 (Uesugi et al., Science (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., Cell (1997) 91:741-752).

C. Structure of the hTR\$ LBD:GRIP1 NR-box 2 peptide interface

The hTRß LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are I280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

The GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but

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defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTRB LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

Example 18: Overall Structure of the DES-hER\alpha-LBD-NR-box 2 Peptide Complex

The asymmetric unit of the DES-hERa LBD-NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E2 and RAL (Brzozowski, et al., supra and Tanenbaum, et al., supra). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar structures (r.m.s.d. 0.47 Å based on Ca positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E2 (Brzozowski, et al., supra); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix. Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

Example 19: Structure of the OHT-hERa LBD Complex

The binding of OHT induces a conformation of the hERa LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES

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complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., supra).

Example 20: Coactivator binding site structure and function

A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., Figures 5, 14, and 15). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453, L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational change upon hormone binding included Leu454 and Glu457. Thus, the site identified by

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mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ERα LBD buries 1000 Ų of predominantly hydrophobic surface area from both molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization of the binding site of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ERα LBD, which is the same NR-box 2 peptide utilized to crystallize the T₃-TR

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LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter. These residues are highly conserved among the nuclear receptor super family (Figure 19). Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of exploiting the slight differences among the coactivator binding sites of nuclear receptors in designing and identifying compounds that target specific nuclear receptors.

The ERα LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) α helix formed by the side chains of Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689 and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile 689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix project away from the ERα receptor and either interact predominantly with solvent or form symmetry contacts. None of the side chains of the polar and charged residues outside the helical region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is involved in hydrogen bonds or salt bridges with its associated ERα LBD monomer. The ε-amino group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-terminal three residues of peptide B are displaced from monomer B and interact extensively with a symmetry-related ERα LBD.

In addition to interacting with the hydrophobic face of the peptide helix, the ER α LBD stabilizes the main chain conformation of the NR box peptide by forming capping interactions with both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These interactions position the stabilizing charges of the γ -carboxylate of Glu 542 and ϵ -amino group of Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542

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hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the ε-amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

Except for the orientation of helix 12, the structure of the peptide binding groove of the ER α LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its ϵ -amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu 380. The Glu 380 γ -carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER α LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the

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5 OHT complex buries more solvent accessible surface area (~1200 Ų) than the NR box peptide in the DES-ERα LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator proteins to nuclear receptors for all members of the nuclear receptor super family.

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25

All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

PCT/US99/06899 WO 99/060014

Appendix 1 5

Atomic Coordinates for Human TR-B Complexed With T3, and a GRIP1 NR-box 2 Peptide

```
REMARK full length numbering
    REMARK all residue names correct
10
    REMARK peptide sequence
    REMARK two molecules of TRB - CHAIN A and CHAIN B
    REMARK two molecules of T3 - CHAIN J and CHAIN K
    REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y
    REMARK chain X lies between A and B
15
    REMARK chain Y interacts with B only
    REMARK residues differing between A and B include:
    REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains)
    REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains)
    REMARK additionally Gly 261, Gly 262 are not visible in chain A
20
    REMARK residues differing between X and Y include:
    REMARK A 692 Arg
    REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698
    REMARK are not visible in chain Y
                                                                         7
                                    52.546 23.912
                                                            1.00 45.76
                                                    35.239
                     LYS A 211
              1 N
25
    MOTA
                                                    36.586
                                                            1.00 43.42
                                                                         6
                                    52.944 24.345
              2 CA LYS A 211
    MOTA
                                                            1.00 35.68
                                                                         6
                                    52.035 23.665
                                                   37.836
                     LYS A 211
              3 C
    MOTA
                                                            1.00 33.58
                                                                         8
                                    51.511 22.556
                                                   37.763
                     LYS A 211
              4 0
    MOTA
                                                                         6
                                                    36.779
                                                            1.00 46.72
                                    52.610
                                           25.825
                    LYS A 211
              5 CB
    MOTA
                                                                         7
                                    51.678 24.182
                                                    39.199
                                                            1.00 35.64
              6 N
                     PRO A 212
30
    MOTA
                                                                         6
                                                   39.842
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                                    52.082 25.474
              7 CD
                     PRO A 212
     MOTA
                                    50.809 23.379 40.166 1.00 38.35
                                                                         6
                     PRO A 212
     MOTA
              8 CA
                                                   41.440 1.00 38.95
                                           24.194
                                    50.670
              9 CB
                     PRO A 212
     MOTA
                                                    41.255 1.00 42.00
                                                                         6
                                    51.455
                                            25.469
                    PRO A 212
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                                    49.433 23.097
             11 C
                     PRO A 212
35
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                     PRO A 212
             12 0
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                                                            1.00 40.31
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     MOTA
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                     GLU A 213
     MOTA
             14 CA
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                                                                         6
                     GLU A 213
             15
                 CB
     MOTA
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                                                            1.00 47.60
                                                                         6
                     GLU A 213
 40
                 CG
     MOTA
             16
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                                                            1.00 50.68
                                                                         6
                                                    36.353
                     GLU A 213
              17
                 CD
     MOTA
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                                     49.355 18.547
                                                    36.474
                 OE1 GLU A 213
     MOTA
              18
                                                            1.00 49.06
                                     49.356 20.368
                                                    35.180
              19 OE2 GLU A 213
     MOTA
                                                                          6
                                                            1.00 45.96
                                            20.988
                                                    40.747
                      GLU A 213
                                     46.711
              20 C
     ATOM
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                                                                          8
                                                     41.910
                                     47.111 21.136
                      GLU A 213
 45
              21 0
     MOTA
                                                                          7
                                                            1.00 46.52
                                                    40.515
                      PRO A 214
                                     45.463 20.460
              22 N
     MOTA
                                                            1.00 46.44
                                     44.985 20.184
                                                    39.148
              23
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                    PRO A 214
     MOTA
                                                            1.00 47.52
                                                                          6
                                     44.447 20.124
                                                     41.596
                     PRO A 214
              24
                 CA
     MOTA
                                                    40.816
                                                            1.00 45.40
                                                                          6
                                     43.249 19.629
                     PRO A 214
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     MOTA
                                                     39.327
                                                            1.00 49.89
                                                                          6
                                     43.588 19.674
              26 CG PRO A 214
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     MOTA
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                                                     42.625
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                                     44.787 19.082
                      PRO A 214
              27 C
     MOTA
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                                                             1.00 44.49
                                     45.816 18.466
              28 0
                      PRO A 214
     ATOM
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                                                             1.00 45.24
                                     43.915 18.876
                                                     43.606
                      THR A 215
              29 N
     MOTA
                                                             1.00 49.36
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                                                     44.686
                                     44.161 17.890
              30 CA THR A 215
     MOTA
                                                                          6
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                                     44.163 18.586 46.093
                      THR A 215
 55
              31 CB
     MOTA
                                                     46.728
                                                             1.00 52.26
                                                                          8
                                     42.878 18.447
              32
                 OG1 THR A 215
     ATOM
                                                     45.974
                                                             1.00 39.43
                                                                          6
              33 CG2 THR A 215
                                     44.514 20.031
     MOTA
                                     42.934 16.995 44.667
                                                             1.00 52.51
                                                                          6
                      THR A 215
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MOTA

34 C

								44.691	9 6 6 5 18 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	_
5	MOTA	35	0	THR A		41.81			1.00 53.48	8
	ATOM	36	N	ASP A		43.11		44.607	1.00 58.81	7
	ATOM	37	CA	ASP A		41.97		44.615	1.00 61.51	6
	MOTA	38	CB	ASP A		42.38		45.343	1.00 70.57	6
	ATOM	39	CG	ASP A		42.39		44.475	1.00 78.07	6
10	ATOM	40	OD1	ASP A	216	41.53		43.586	1.00 82.31	8
	MOTA	41	OD2	ASP A	216	43.29		44.684	1.00 86.55	8
	MOTA	42	С	ASP A	216	40.64		45.268	1.00 58.42	6
	MOTA	43	0	ASP A	216	39.59		44.924	1.00 56.85	8
	MOTA	44	N	GLU A	217	40.67		46.217	1.00 54.92	7
15	ATOM	45	CA	GLU A	217	39.50		46.856	1.00 53.37	6
	ATOM	46	CB	GLU A	217	39.94		48.216	1.00 51.02	6
	ATOM	47	С	GLU A	217	39.11	.3 18.144	45.956	1.00 53.55	6
	MOTA	48	0	GLU A	217	37.90		45.695	1.00 54.33	8
	MOTA	43	N	GLU A	218	40.16	18.895	45.511	1.00 49.20	7
20	MOTA	50	CA	GLU A	218	39.93	33 20.073	44.661	1.00 45.94	6
	ATOM	51	CB	GLU A	218	41.23	32 20.855	44.304	1.00 43.43	6
	MOTA	52	CG	GLU A	218	41.90	21.579		1.00 40.86	6
	MOTA	53	CD	GLU A	218	43.06	51 22.446		1.00 39.88	6
	MOTA	54	OE1	GLU A	218	43.89	22.019		1.00 37.61	8
25	ATOM	55	OE2	GLU A	218	43.18	33 23.583	45.599	1.00 34.01	8
	ATOM	56	С	GLU A	218	39.24	19.647	43.390		6
	ATOM	57	0	GLU A	218	38.30	20.291	42.964	1.00 45.31	8
	MOTA	58	N	TRP F	219	39.7	20 18.553	42.797	1.00 44.02	7
	MOTA	59	CA	TRP F	A 219	39.1	09 18.061		1.00 46.97	6
30	MOTA	60	СВ	TRP F	1 219	39.7	99 16.793		1.00 48.42	6
	ATOM	61	CG	TRP A	1 219	40.8			1.00 54.61	6
	MOTA	62	CD2	TRP A	1 219	40.7			1.00 55.24	6
	MOTA	63	CE2	TRP A	A 219	42.0			1.00 53.67	6
	MOTA	64	CE3	TRP A	A 219	39.6			1.00 54.55	6
35	MOTA	65	CD1	TRP A	A 219	42.1			1.00 55.75	6
	MOTA	66	NE]	TRP A	A 219	42.8			1.00 54.43	7
	MOTA	67	CZ2	TRP	A 219	42.3			1.00 52.54	6
	MOTA	68	CZ3	3 TRP 2	A 219	39.9			1.00 55.17	6
	MOTA	69	CH2	TRP	A 219	41.2				6
40	MOTA	70	С		A 219	37.6				6
	MOTA	71	0		A 219	36.7				8
	MOTA	72	N	GLU	A 220	37.3				7
	ATOM	73	CA		A 220	36.0				6
	MOTA	74	CB		A 220	36.0				6
45	ATOM	75	CG		A 220	35.1				6
	ATOM	76			A 220	35.7				6
	ATOM	77	OE	l GLU		36.8				8
	MOTA	78	OE:		A 220	35.0				8
	MOTA	79	C		A 220	35.1				6
50	MOTA	80	0		A 220	33.9				8
	MOTA	81	N		A 221	35.7				7
	ATOM	82	CA		A 221	35.0				6
	MOTA	83	CB		A 221	35.9				6
	ATOM	8 4			A 221	35.3				6
55	MOTA	85		1 LEU		33.9				6
	MOTA	86	CD	2 LEU		36.2				6
	MOTA	87	C		A 221	34.5				6
	MOTA	88	0	LEU	A 221	33.3	392 21.10	4 42.395	1.00 45.25	8

									_			
5	MOTA	89	N	ILE .	A	222	35.498	20.871	41.628		39.09	7
	ATOM	90	CA	ILE .	A	222	35.192	21.226	40.254		35.47	6
	MOTA	91	CB	ILE	A	222	36.379	20.997	39.343		33.74	6
	MOTA	92	CG2	ILE	A	222	35.970	21.182	37.893		28.86	6
	MOTA	93	CG1	ILE	A	222	37.532	21.922	39.707		33.33	6
10	MOTA	94	CD1	ILE	Α	222	38.804	21.586	39.004		34.85	6
	MOTA	95	С	ILE	A	222	34.067	20.365	39.735		34.26	6
	MOTA	96	0	ILE	Α	222	33.033	20.873	39.319	1.00	31.90	8
	MOTA	97	N	LYS	A	223	34.301	19.058	39.750	1.00	39.49	7
	MOTA	98	CA	LYS	Α	223	33.316	18.100	39.276	1.00	44.43	6
15	ATOM	99	CB	LYS	A	223	33.603	16.713	39.852	1.00	50.81	6
	ATOM	100	CG	LYS	Α	223	32.741	15.631	39.227	1.00	62.51	6
	ATOM	101	CD	LYS	A	223	32.859	14.291	39.943	1.00	72.22	6
	ATOM	102	CE	LYS			31.798	13.318	39.430	1.00	74.55	6
	MOTA	103	NZ	LYS	Α	223	31.900	11.985	40.106	1.00	75.78	7
20	ATOM	104	С	LYS			31.913	18.565	39.681	1.00	42.81	6
	MOTA	105	0	LYS			30.936	18.323	38.984	1.00	40.36	8
	ATOM	106	N	THR			31.849	19.236	40.833	1.00	39.89	7
	ATOM	107	CA	THR			30.602	19.792	41.378	1.00	39.93	6
	ATOM	108	СВ	THR			30.805	20.206	42.851	1.00	40.57	6
25	ATOM	109	OG1	THR			31.330	19.113	43.616	1.00	39.27	8
	MOTA	110	CG2	THR			29.500	20.684	43.461	1.00	38.11	6
	MOTA	111	С	THR			30.167	21.011	40.533	1.00	39.96	6
	MOTA	112	0	THR			29.313	20.899	39.655	1.00	36.67	8
	ATOM	113	N	VAL			30.777	22.160	40.832		38.02	7
30	ATOM	114	CA	VAL			30.532	23.426	40.137	1.00	38.12	6
	ATOM	115	CB	VAL			31.797	24.292	40.122	1.00	38.19	6
	ATOM	116	CG1	VAL			31.512	25.636	39.491	1.00	36.77	6
	ATOM	117	CG2	VAL			32.343	24.464	41.505	1.00	41.76	6
	ATOM	118	C	VAL			30.070	23.195	38.706	1.00	37.52	6
35	ATOM	119	0	VAL			29.119	23.803	38.239	1.00	36.77	8
	ATOM	120	N			226	30.783	22.316	38.018	1.00	34.02	7
	ATOM	121	CA			226	30.489	21.971	36.636	1.00	34.67	6
	MOTA	122	CB	THR	Α	226	31.565	20.999	36.083	1.00	30.56	6
	ATOM	123	OG1	THR	Α	226	32.805	21.696	35.889	1.00	32.20	8
40	ATOM	124	CG2	THR	Α	226	31.108	20.346	34.783	1.00	20.99	6
	ATOM	125	С	THR	Α	226	29.100	21.361	36.510	1.00	36.41	6
	ATOM	126	0	THR	Α	226	28.255	21.877	35.785	1.00	39.64	8
	ATOM	127	N			227	28.880	20.260	37.222	1.00	39.20	7
	ATOM	128	CA	ALA	Α	227	27.602	19.562	37.204	1.00	36.93	6
45	MOTA	129	СВ			227	27.526	18.600	38.381	1.00	38.06	6
	ATOM	130	С	ALA	Α	227	26.507	20.604	37.318	1.00	37.69	6
	MOTA	131	0			227	25.444	20.489	36.718	1.00	40.94	8
	MOTA	132	N			228	26.811	21.630	38.107	1.00	32.86	7
	MOTA	133	CA			228	25.903	22.734	38.356	1.00	32.48	6
50	ATOM	134	СВ			228	26.448	23:587	39.486	1.00	28.25	6
	ATOM	135	С			228	25.732	23.570	37.101	1.00	36.12	6
	ATOM	136	0			228	24.673	23.560	36.473		37.86	8
	ATOM	137	N			229	26.782	24.306	36.752		33.58	7
	ATOM	138	CA			229	26.762	25.158	35.585		32.97	6
55	ATOM	139	СВ			229	28.155	25.691	35.266		33.69	6
	ATOM	140	CG			229	28.250	26.333	33.929		28.39	6
	ATOM	141		HIS			29.025	26.081	32.838		28.83	6
	ATOM	142		HIS			27.386	27.368	33.542		30.47	7

_		7.63	CEI	HIS A	229	27.654	27.692	32.280	1.00 26.95	6
5	ATOM	143		HIS A		28.635			1.00 31.27	7
	MOTA	144 145		HIS A		26.225	24.541	34.312	1.00 38.40	6
	MOTA	145		HIS A		25.591	25.227	33.528	1.00 41.49	8
	ATOM	147		VAL A		26.519	23.256	34.113	1.00 38.55	7
10	MOTA		CA	A LAV		26.088	22.554	32.916	1.00 40.40	6
10	MOTA	148 149	CB	VAL A		26.890	21.256	32.701	1.00 44.68	6
	ATOM			VAL A		26.557	20.656	31.345	1.00 39.39	6
	ATOM	150		VAL A		28.381	21.509	32.817	1.00 42.18	6
	ATOM	151 152	C	VAL A		24.603	22.239	32.900	1.00 44.28	6
1.5	ATOM	152	0	VAL A		23.959	22.316	31.847	1.00 45.94	8
15	MOTA	153	N	ALA A		24.072	21.862	34.059	1.00 45.59	7
	ATOM .	155	CA	ALA A		22.669	21.500	34.175	1.00 47.84	6
	ATOM .	156	CB	ALA A		22.482	20.582	35.374	1.00 45.08	6
	MOTA	157	C	ALA A		21.792	22.734	34.314	1.00 48.04	6
20	ATOM	158	0	ALA A		20.565	22.647	34.324	1.00 49.95	8
20	ATOM	159	N	THR A		22.436	23.894	34.384	1.00 47.26	7
	ATOM	160	CA	THR A		21.722	25.161	34.528	1.00 43.64	6
	MOTA	161	CB	THR A		22.112	25.832	35.850	1.00 41.93	6
	ATOM	162	OG1	THR A		23.467	26.283	35.791	1.00 39.10	8
25	MOTA	163	CG2	THR P		21.990	24.846	37.008	1.00 29.80	6
25	MOTA	164	C	THR F		22.055	26.114	33.387	1.00 43.97	6
	MOTA	165	Ō	THR F		21.679	27.279	33.436	1.00 40.55	8
	MOTA	166	N	ASN A		22.783	25.625	32.381	1.00 48.62	7
	MOTA	167	CA	ASN A	A 233	23.134	26.468	31.231	1.00 58.62	6
30	ATOM	168	CB	ASN A		24.626	26.283	30.880	1.00 62.44	6
	MOTA	169	CG	ASN A		25.141	27.355	29.927	1.00 68.35	6 8
	MOTA	170		ASN A		24.822	28.544	30.096	1.00 65.50 1.00 74.29	7
	MOTA	171		ASN A		25.951	26.951	28.959	1.00 74.29	6
	MOTA	172	С		A 233	22.241	26.035	30.073 29.604	1.00 69.47	8
35	ATOM	173	0		A 233	22.312	24.900 26.954	29.646	1.00 68.80	7
	MOTA	174	N		A 234	21.381 20.423	26.708	28.564	1.00 70.98	6
	MOTA	175	CA		A 234	19.748	28.015	28.186	1.00 71.43	6
	MOTA	176	CB		A 234	20.988	26.062	27.308	1.00 73.83	6
4.0	MOTA	177	C		A 234 A 234	22.041	26.419	26.822	1.00 74.33	8
40	ATOM	178	О И		A 235	20.227	25.096	26.819	1.00 75.07	7
	ATOM	179 180			A 235	20.562	24.363	25.629	1.00 76.32	6
	MOTA				A 235	20.328	25.239	24.391	1.00 76.98	6
	MOTA	181 182			A 235	18.887		23.908	1.00 77.07	6
15	ATOM	183			A 235	17.896		25.019		6
45	ATOM ATOM	184			A 235	17.668		25.768		8
	ATOM	185			A 235	17.313		25.149		7
	ATOM	186			A 235	21.960		25.573	1.00 77.15	6
	ATOM	187			A 235	22.386		24.508		
50	MOTA	188			A 236	22.676		26.687	1.00 77.46	
30	ATOM	189			A 236	24.053			1.00 78.37	
	ATOM	190			A 236	24.923		25.390		
	ATOM	191			A 236	24.917		24.844		
	MOTA	192			A 237	25.739				
55		193			A 237	26.566	22.760			
	ATOM	194			A 237	27.981				
	ATOM	195			A 237	28.821				
	ATOM	196	6 C	SER	A 237	25.938	22.127	22.542	1.00 75.35	6

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5	ATOM	197	0	SER	A	237	26.605	21.418	21.797	1.00	75.47	8
	ATOM	198	N	HIS	A	238	24.648	22.410	22.353	1.00	75.56	7
	ATOM	199	CA	HIS	A	238	23.842	21.981	21.236	1.00	75.46	6
	ATOM	200	CB	HIS	A	238	22.990	20.732	21.661	1.00	75.85	6
	ATOM	201	CG	HIS	A	238	22.408	19.933	20.542	1.00	40.00	6
10	ATOM	202	CD2	HIS	А	238	22.790	18.757	19.957	1.00	40.00	6
	ATOM	203	ND1	HIS	Α	238	21.223	20.303	19.875	1.00	40.00	. 7
	ATOM	204		HIS			20.951	19.365	18.953	1.00		6
	ATOM	205		HIS			21.874	18.444	18.994	1.00	40.00	7
	ATOM	206	С	HIS			22.971	23.284	20.964	1.00	74.10	6
15	ATOM	207	0	HIS			21.863	23.137	20.441		75.34	8
	ATOM	208	N	TRP			23.487	24.510	21.368		73.39	7
	ATOM	209	CA	TRP			22.872	25.894	21.195		74.02	6
	ATOM	210	CB	TRP			23.563	27.026	22.005		81.77	6
	ATOM	211	CG			239	25.022	27.366	21.688		89.67	6
20	ATOM	212	CD2	TRP			25.532	28.662	21.240	1.00		6
	ATOM	213	CE2	TRP			26.961	28.522	21.136		95.46	6
	MOTA	214	CE3	TRP	Α	239	24.936	29.911	20.969		95.35	6
	ATOM	215	CD1	TRP	Α	239	26.102	26.548	21.781		94.16	6
	ATOM	216	NE1	TRP			27.268	27.241	21.475		97.48	7
25	ATOM	217	CZ2	TRP	Α	239	27.798	29.598	20.764	1.00		6
	MOTA	218	CZ3	TRP	A	239	25.763	30.967	20.569	1.00		6
	ATOM	219	CH2	TRP	Α	239	27.171	30.825	20.482	1.00		6
	ATOM	220	С	TRP	A	239	22.799	26.407	19.774	1.00	70.77	6
	ATOM	221	0	TRP	Α	239	21.706	26.562	19.263	1.00	71.70	8
30	MOTA	222	N	LYS	A	240	23.946	26.701	.19.157	1.00	67.10	7
	ATOM	223	CA	LYS	A	240	23.978	27.180	17.783	1.00	65.63	6
	ATOM	224	CB	LYS	Α	240	25.314	26.780	17.153	1.00	66.65	6
	MOTA	225	CG	LYS	A	240	26.529	27.342	17.872	1.00	69.83	6
	MOTA	226	CD			240	27.805	27.037	17.108		71.49	6
35	MOTA	227	CE			240	28.980	27.720	17.776		71.31	6
	MOTA	228	NZ			240	30.238	27.438	17.034		72.23	7
	MOTA	229	С			240	22.808	26.699	16.895		66.19	6
	MOTA	230	0			240	22.550	27.298	15.851		65.20	8
	MOTA	231	N			241	22.113	25.640	17.325		66.69	7
40	ATOM	232	CA			241	20.976	25.078	16.599	1.00		6
	ATOM	233	CB			241	21.122	23.562	16.550		67.98	6
	MOTA	234	CG			241	22.304	23.121	15.693		70.19	6
	ATOM	235		ASN			22.404	23.506	14.503		71.37	8
4 5	ATOM	236		ASN			23.176	22.310	16.271		71.48	7
45	MOTA	237	C			241	19.570	25.421	17.152		66.62	6
	ATOM	238	0			241	18.581	24.822	16.731		64.76	8
	ATOM	239	N			242	19.475	26.380	18.069		66.86	7
	ATOM	240	CA			242	18.191	26.786	18.642		67.46	6
50	ATOM	241	CB			242	18.164	26.396	20.119		67.93	6
50	ATOM	242	CG			242	18.250	24.896	20.337		71.52	6
	ATOM	243	CD			242	17.004	24.149	19.821		74.32	6
	MOTA	244	CE			242	15.755	24.491	20.643		74.41	6
	ATOM	245	ΝZ			242	15.927	24.161	22.109		74.44	7
E	ATOM	246	C			242	18.143	28.291	18.483		66.28	6
55	ATOM	247	0			242	17.102	28.923	18.592		67.61	8
	MOTA	248	N			243	19.334	28.813	18.204		64.19	7
	MOTA	249	CA			243	19.617	30.219	17.975		62.43	6
	MOTA	250	CB	ARG	A	243	21.070	30.274	17.463	1.00	60.12	6

5	ATOM	251		ARG A		21.665	31.636	17.305	1.00 40.00	6
	ATOM	252	CD	ARG A	243	23.213	31.599	17.267	1.00 40.00	6
	ATOM	253	NE	ARG A	243	23.826	31.217	15.996	1.00 40.00	7
	ATOM	254	CZ	ARG A	243	25.113	31.439	15.714	1.00 40.00	6
	ATOM	255	NHl	ARG A	243	25.905	32.041	16.616	1.00 40.00	7
10	MOTA	256	NH2	ARG A	243	25.592	31.097	14.520	1.00 40.00	7
	ATOM	257	С	ARG A	243	18.639	30.789	16.950	1.00 62.97	6
	ATOM	258	0	ARG A	243	18.662	30.390	15.784	1.00 63.96	8
	ATOM	259	N	LYS A	244	17.771	31.692	17.393	1.00 62.41	7
	ATOM	260	CA	LYS A	244	16.790	32.309	16.498	1.00 61.57	6
15	ATOM	261	CB	LYS A	244	15.368	31.974	16.962	1.00 63.68	6
	ATOM	262	CG	LYS A	244	15.102	30.471	17.104	1.00 71.29	6
	ATOM	263	CD	LYS A	244	13.641	30.167	17.468	1.00 73.83	6
	ATOM	264	CE	LYS A	244	13.182	30.908	18.737	1.00 74.71	6
	ATOM	265	NZ	LYS A		13.951	30.536	19.970	1.00 73.32	7
20	ATOM	266	С	LYS A		17.009	33.806	16.501	1.00 59.30	6
	ATOM	267	0	LYS A		16.562	34.514	17.399	1.00 56.34	8
	ATOM	268	N	PHE A		17.705	34.264	15.468	1.00 57.06	7
	ATOM	269	CA	PHE A		18.045	35.692	15.333	1.00 59.01	6
	ATOM	270	СВ	PHE A		18.825	35.947	14.049	1.00 59.62	6
25	ATOM	271	CG	PHE A		19.908	34.979	13.834	1.00 66.60	6
	ATOM	272	CD1	PHE A		19.618	33.714	13.399	1.00 67.17	6
	ATOM	273	CD2	PHE A		21.198	35.309	14.139	1.00 69.25	6
	ATOM	274	CEl	PHE A		20.614	32.794	13.255	1.00 69.92	6
	ATOM	275	CE2	PHE A		22.189	34.385	13.994	1.00 70.50	6
30	ATOM	276	CZ	PHE A		21.897	33.126	13.552	1.00 70.89	6
	ATOM	277	С	PHE A		16.856	36.620	15.340	1.00 60.68	6
	ATOM	278	0	PHE A		15.946	36.516	14.528	1.00 62.37	8
	ATOM	279	N	LEU A	246	16.919	37.558	16.272	1.00 60.10	7
	ATOM	280	CA	LEU A	246	15.884	38.554	16.437	1.00 59.44	6
35	ATOM	281	СВ	LEU A	246	16.227	39.510	17.585	1.00 57.43	6
	ATOM	282	CG	LEU A	246	15.100	40.384	18.086	1.00 54.41	6
	ATOM	283	CD1	LEU A	246	14.010	39.474	18.640	1.00 52.43	6
	ATOM	284	CD2	LEU A	246	15.575	41.325	19.151	1.00 51.69	6
	ATOM	285	С	LEU A	246	15.717	39.330	15.135	1.00 62.05	6
40	MOTA	286	0	LEU A	246	16.706	39.609	14.430	1.00 59.85	8
	MOTA	287	N	PRO A	247	14.473	39.668	14.784	1.00 63.33	7
	ATOM	288	CD	PRO A	247	13.263	39.314	15.534	1.00 64.44	6
	ATOM	289	CA	PRO A	247	14.198	40.421	13.558	1.00 63.56	6
	ATOM	290	CB	PRO A	247	12.687	40.671	13.600	1.00 64.42	6
45	MOTA	291	CG	PRO A	247	12.161	39.922	14.729	1.00 64.90	6
	ATOM	292	С	PRO A	247	14.996	41.733	13.496	1.00 61.94	6
	ATOM	293	0	PRO A	247	15.159	42.455	14.486	1.00 61.60	8
	ATOM	294	N	GLU A	248	15.506	42.006	12.299	1.00 61.33	7
	ATOM	295	CA	GLU A	248	16.280	43.197	11.976	1.00 63.50	6
50	ATOM	296	CB	GLU A	248	16.481	43.273	10.437	1.00 66.94	6
	ATOM	297	CG	GLU A	248	17.012	44.671	9.966	1.00 68.70	6
	ATOM	298	CD	GLU A	248	16.981	44.939	8.471	1.00 40.00	6
	ATOM	299	OE1	GLU A	248	16.432	44.144	7.644	1.00 40.00	8
	ATOM	300	OE2	GLU A	248	17.509	46.015	8.086	1.00 40.00	8
55	ATOM	301	С	GLU A		15.624	44.489	12.458	1.00 64.19	6
	ATOM	302	0	GLU A	248	16.298	45.395	12.918	1.00 65.56	8
	ATOM	303	N	ASP A		14.300	44.545	12.323	1.00 64.36	7
	ATOM	304	CA	ASP A	249	13.493	45.703	12.673	1.00 63.33	6

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5	ATOM	305	CB	ASP 3			12.088	45.531	12.116		62.97	6
	ATOM	306	CG	ASP :			11.277	44.527	12.870		64.63	6
	MOTA	307		ASP :			11.687	43.352	12.963		64.84	8
	ATOM	308		ASP .			10.183	44.880	13.395		66.52	8
10	ATOM	309	С	ASP .			13.371	46.062	14.130		64.31	6
10	ATOM	310	0	ASP .			13.310	47.250	14.468		64.73	8
	MOTA	311	Ŋ	ILE .			13.274	45.049	14.997		63.09	7
	MOTA	312	CA	ILE			13.133	45.318	16.418		64.39	6
	ATOM	313	CB	ILE			13.035	44.034	17.214		65.79	6
	MOTA	314	CG2	ILE			12.001	44.104	18.336		64.78	6
15	MOTA	315	CG1	ILE			12.611	42.860	16.341		65.28	6
	MOTA	316	CD1	ILE			11.753	41.852	17.088		65.08	6
	MOTA	317	С	ILE			14.404	46.104	17.276		65.21	6
	MOTA	318	0	ILE			15.155	45.506	18.047		64.05	8
	ATOM	319	N	GLY			14.670	47.529	17.299		65.48	7
20	MOTA	320	CA	GLY			15.871	48.326	18.042		67.32	6
	MOTA	321	С	GLY			16.595	49.110	16.895		68.52	6
	MOTA	322	0	GLY			17.528	48.616	16.266		65.49	8
	MOTA	323	Ŋ	GLN			16.162	50.356	16.557		72.26	7
	MOTA	324	CA	GLN			16.541	50.930	15.207		74.10	6
25	MOTA	325	CB	GLN			15.316	50.844	14.295		75.82	6
	MOTA	326	С	GLN			16.995	52.403	15.084			6
	MOTA	327	0	GLN			17.572	52.955	15.986	1.00	76.50	8
	MOTA	328	N	ALA			16.374	53.372	13.908		80.78	7
	MOTA	329	CA	ALA			16.687	54.725	13.567		83.70	6
30	MOTA	330	CB	ALA			16.381	54.956	12.093		83.23	6
	MOTA	331	С	ALA			16.159	55.960	14.345		85.59	6
	MOTA	332	0	ALA			15.317	56.721	13.798		85.69	8
	ATOM	333	N	PRO			16.384	56.155	16.264		35.05	7
	ATOM	334	CD	PRO			17.102	55.053	16.908		33.97	6
35	MOTA	335	CA	PRO			16.002	57.231	17.219		35.89	6
	MOTA	336	CB	PRO			16.534	56.756	18.563		33.94	6
	ATOM	337	CG	PRO			17.146	55.441	18.349		33.31	6
	ATOM	338	С	PRO			16.717	58.498	16.731		37.75	6
4.0	MOTA	339	0	PRO	A	254	17.838	58.804	17.100	1.00	38.78	8
40	TER	_			_							
	MOTA	1	N	LYS			18.045	57.462	23.875		61.71	7
	MOTA	2	CA	LYS			16.824	56.712	24.215		64.36	6
	MOTA	3	CB	LYS			15.758	57.004	23.141		63.50	6
4.5	MOTA	4	C	LYS			16.841	55.180	24.429		63.41	6
45	MOTA	5	0	LYS			17.877	54.542	24.409		61.93	8
	MOTA	6	N	VAL			15.615	54.664	24.654		61.15	7
	ATOM	7	CA	VAL			15.292	53.229	24.856		59.46	6
	MOTA	8	CB	VAL			14.251	52.974	25.978		59.03	6
	MOTA	9	CG1				14.229	51.494	26.368		53.79	6
50	ATOM	10	CG2				14.449	53.818	27.142		55.32	6
	ATOM	11	С	VAL			14.590	52.820	23.554		60.96	6
	ATOM	12	0	VAL			14.734	53.468	22.508		62.13	8
	MOTA	13	N	ASP			13.802	51.755	23.634		62.59	7
	MOTA	14	CA	ASP			12.995	51.263	22.526		64.95	6
55	MOTA	15	CB	ASP			13.825	51.077	21.271		64.32	6
	MOTA	16	CG	ASP			13.282	50.048	20.485		67.70	6
	MOTA	17		ASP			12.795	50.011	19.446		72.59	8
	ATOM	18	OD2	ASP	A	265	13.354	48.867	20.294	1.00	68.84	8

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5	ATOM	19 C ASP A 265		9.943		1.00 65.64	6
,	ATOM	20 O ASP A 265		3.850		1.00 68.81	8
	ATOM	21 N LEU A 266	11.256 50	0.152	23.702	1.00 65.12	7
	ATOM	22 CA LEU A 266	10.368 49	9.169	24.288	1.00 63.40	6
	ATOM	23 CB &EU A 266	9.115 49	9.938	24.708	1.00 67.34	6
10	ATOM	24 CG LEU A 266	9.399 53	1.124	25.618	1.00 69.35	6
10		25 CD1 LEU A 266		2.148	25.533	1.00 68.24	6
	ATOM	26 CD2 LEU A 266		0.631	27.021	1.00 70.47	6
	MOTA			7.888	23.559	1.00 59.67	6
	ATOM			6.879	24.220	1.00 53.35	8
	MOTA		• •	7.904	22.235	1.00 58.01	7
15	ATOM	_ ·		6.682	21.572	1.00 58.34	6
	MOTA			6.855	20.048	1.00 59.21	6
	MOTA			5.494	19.322	1.00 62.89	6
	MOTA	32 CG GLU A 267		5.592	17.883	1.00 67.66	6
	MOTA	33 CD GLU A 267		6.263	17.080	1.00 69.95	8
20	MOTA	34 OE1 GLU A 267		4.974	17.503	1.00 69.40	8
	ATOM	35 OE2 GLU A 267		15.683	21.895	1.00 57.67	6
	MOTA	36 C GLU A 267		14.485	21.988	1.00 58.34	8
	MOTA	37 O GLU A 267		16.222	22.054	1.00 53.43	7
	MOTA	38 N ALA A 268		45.454	22.374	1.00 49.00	6
25	MOTA	39 CA ALA A 268		46.241	21.983	1.00 45.72	6
	MOTA	40 CB ALA A 268		45.196	23.873	1.00 45.76	6
	MOTA	41 C ALA A 268		44.042	24.307	1.00 41.50	8
	ATOM	42 O ALA A 268		46.277	24.663	1.00 41.43	7
	MOTA	43 N PHE A 269	- -: -	46.158	26.118	1.00 43.96	6
30	MOTA	44 CA PHE A 269		47.426	26.777	1.00 40.10	6
	ATOM	45 CB PHE A 269		47.345	28.271	1.00 40.44	6
	MOTA	46 CG PHE A 269		47.595	29.034	1.00 38.98	6
	MOTA	47 CD1 PHE A 269		46.946	28.903	1.00 37.15	6
	MOTA	48 CD2 PHE A 269		47.469	30.436	1.00 32.12	6
35	ATOM	49 CE1 PHE A 269	-	46.815	30.303	1.00 38.41	6
	MOTA	50 CE2 PHE A 269		47.070		1.00 40.55	6
	MOTA	51 CZ PHE A 269		45.012		1.00 49.76	6
	MOTA	52 C PHE A 269	12.017 12.277	44.324		1.00 52.15	8
	MOTA	53 O PHE A 269	10.934	44.835		1.00 53.15	7
40	MOTA	54 N SER A 270	9.988	43.768			6
	ATOM	55 CA SER A 270	8.727	43.943			6
	ATOM	56 CB SER A 270	7.785	42.918			8
	MOTA	57 OG SER A 270	10.637	42.464			6
	MOTA	58 C SER A 270	11.068	41.741			8
45		59 O SER A 270	10.683	42.173			7
	MOTA	60 N HIS A 271	11.276	40.932			6
	MOTA	61 CA HIS A 271		41.118			6
	MOTA	62 CB HIS A 271	11.797	40.885			6
	ATOM	63 CG HIS A 271	10.775	39.89			6
50	ATOM	64 CD2 HIS A 271	10.633				7
	MOTA	65 ND1 HIS A 271	9.673	41.73			6
	MOTA	66 CE1 HIS A 271	8.936	41.24			7
	MOTA	67 NE2 HIS A 271	9.495	40.13			6
	MOTA	68 C HIS A 271	12.402	40.41			8
55	MOTA 6	69 O HIS A 271	12.707	39.22			7
	MOTA	70 N PHE A 272	13.029	41.33			
	ATOM	71 CA PHE A 272	14.130	41.00			
	MOTA	72 CB PHE A 272	15.077	42.19	4 26.51	2 1.00 30.07	•

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5	71 077 037	77	~~						
,	ATOM	73		PHE A 27	•		25.282	1.00 33.39	6
	ATOM	74		PHE A 27	•	43.615	25.093	1.00 33.14	6
	ATOM	75				41.394	24.346		6
	ATOM	76				43.807	23.988		6
10	ATOM	77				41.585	23.244	1.00 43.28	6
10	ATOM	78		PHE A 272	2 17.634	42.786			6
	ATOM	79	С	PHE A 272	2 13.650				6
	ATOM	80	0	PHE A 272	2 14.081				8
	ATOM	81	N	THR A 273				1.00 41.64	7
	ATOM	82	CA	THR A 273				1.00 45.97	
15	ATOM	83	CB	THR A 273		42.025		1.00 45.97	6
	MOTA	84	OG1	THR A 273		42.422	29.859	1.00 31.32	6
	ATOM	85	CG2	THR A 273		43.211	30.565	1.00 49.73	8
	ATOM	86	С	THR A 273		39.731	29.664		6
	ATOM	87	0	THR A 273		39.183	30.680	1.00 46.23	6
20	ATOM	88	N	LYS A 274		39.412	28.440	1.00 41.21	8
	ATOM	89	CA	LYS A 274		38.362	28.211	1.00 46.21	7
	ATOM	90	СВ	LYS A 274		38.405	26.773	1.00 54.53	6
	ATOM	91	С	LYS A 274		37.015	28.515	1.00 54.36	6
	ATOM	92	0	LYS A 274				1.00 56.88	6
25	ATOM	93	N	ILE A 275	- · · - -	36.973	28.759	1.00 57.98	8
	MOTA	94	CA	ILE A 275		35.746	28.491	1.00 56.48	7
	ATOM	95	СВ	ILE A 275		35.346	28.767	1.00 52.64	6
	ATOM	96	CG2	ILE A 275		34.829	27.543	1.00 49.15	6
	ATOM	97	CG1	ILE A 275		36.532	26.429	1.00 47.42	6
30	ATOM	98	CD1	ILE A 275		36.242	27.026	1.00 45.31	6
	ATOM	99	С	ILE A 275		35.870	25.771	1.00 37.22	6
	MOTA	100	0	ILE A 275		34.873	29.982	1.00 51.78	6
	ATOM	101	N	ILE A 276		37.107	30.503	1.00 49.80	8
	MOTA	102	CA	ILE A 276		37.107	30.415	1.00 51.76	7
35	MOTA	103	CB	ILE A 276		38.877	31.537	1.00 52.58	6
	MOTA	104	CG2	ILE A 276		39.340	31.844	1.00 55.04	6
	MOTA	105	CG1	ILE A 276		39.206	32.261	1.00 53.28	6
	MOTA	106				38.942	32.976	1.00 57.31	6
	MOTA	107	С	ILE A 276		36.644	32.655	1.00 60.32	6
40	ATOM	108	Ō	ILE A 276		36.458	32.828	1.00 50.70	6
	ATOM	109	N	THR A 277	13.072	36.209	33.691	1.00 55.55	8
	ATOM	110	CA	THR A 277		35.523	32.963	1.00 47.33	7
	ATOM	111		THR A 277	11.098	35.456	34.158	1.00 42.59	6
	MOTA	112		THR A 277	10.545	36.777	34.217	1.00 44.97	6
45	ATOM	113		THR A 277	10.657	34.838	34.102	1.00 46.38	8
	ATOM	114		THR A 277	13.211	34.118	35.539	1.00 37.17	6
	MOTA	115		THR A 277	13.796	33.796	34.304	1.00 39.84	6
	ATOM	116		PRO A 278	13.055		35.365	1.00 40.55	8
	MOTA	117		PRO A 278	12.370	33.261	33.288	1.00 38.20	7
50	ATOM	118		PRO A 278	13.595	33.534	32.023	1.00 36.34	6
	ATOM	119		PRO A 278	13.153	31.894	33.363	1.00 36.63	6
	ATOM	120		PRO A 278		31.244	32.064	1.00 32.95	6
	ATOM	121		PRO A 278	12.573	32.291	31.239	1.00 35.75	6
	ATOM	122		PRO A 278	15.101	31.932	33.476	1.00 38.60	6
55	ATOM	123		ALA A 279	15.746	30.981	33.898	1.00 37.67	8
-	ATOM	123			15.656	33.051	33.035	1.00 37.05	7
	ATOM	125		ALA A 279	17.087	33.277	33.041	1.00 33.18	6
	ATOM	125		ALA A 279	17.376	34.599	32.348	1.00 30.56	6
		120		ALA A 279	17.624	33.312	34.452	1.00 33.47	6

5	ATOM	127	0	ALA	A 279	18.523	32.555	34.789	1.00 33.74	8
	ATOM	128	N	ILE	A 280	17.060	34.215	35.260	1.00 29.96	7
	ATOM	129	CA	ILE	A 280	17.459	34.362	36.646	1.00 25.94	6
	ATOM	130	CB	ILE	A 280	16.686	35.484	37.315	1.00 26.95	6
	ATOM	131	CG2	ILE	A 280	17.109	35.632	38.733	1.00 15.40	6
10	ATOM	132	CG1	ILE	A 280	16.931	36.808	36.595	1.00 26.73	6
	ATOM	133	CD1		A 280	16.292	38.002	37.272	1.00 34.31	6
	ATOM	134	С		A 280	17.263	33.066	37.412	1.00 31.39	6
	ATOM	135	0		A 280	18.116	32.679	38.207	1.00 35.69	8
	ATOM	136	N		A 281	16.145	32.386	37.165	1.00 30.90	7
15	ATOM	137	CA		A 281	15.854	31.118	37.851	1.00 33.49	6
	ATOM	138	CB		A 281	14.598	30.413	37.277	1.00 33.49	6
	ATOM	139	OG1		A 281	14.795	30.099	35.898	1.00 37.18	8
	ATOM	140	CG2		A 281	13.352	31.281	37.444	1.00 40.45	6
	ATOM	141	С		A 281	17.045	30.176	37.713	1.00 32.83	6
20	ATOM	142	0		A 281	17.478	29.546	38.684	1.00 25.55	8
	ATOM	143	N		A 282	17.561	30.076	36.489	1.00 23.33	7
	ATOM	144	CA		A 282	18.692	29.198	36.218	1.00 32.70	
	ATOM	145	СВ		A 282	19.136	29.374	34.780	1.00 34.27	6
	ATOM	146	ÇG		A 282	19.272	28.086	34.013	1.00 33.78	6
25	ATOM	147	CD		A 282	18.179	27.921	32.977	1.00 43.13	6 6
	ATOM	148	NE		A 282	18.041	29.077	32.117	1.00 58.24	7
	ATOM	149	CZ		A 282	19.018	29.529	31.352	1.00 08.41	6
	MOTA	150	NH1		A 282	20.190	28.886	31.327	1.00 72.31	7
	ATOM	151	NH2		A 282	18.802	30.593	30.595	1.00 77.89	7
30	ATOM	152	С		A 282	19.823	29.582	37.170	1.00 34.81	6
	ATOM	153	0		A 282	20.380	28.735	37.855	1.00 34.01	8
	ATOM	154	N		A 283	20.135	30.882	37.190	1.00 30.03	7
	ATOM	155	CA		A 283	21.171	31.434	38.057	1.00 31.71	6
	ATOM	156	CB		A 283	21.198	32.965	37.981	1.00 29.00	6
35	ATOM	157	CG1		A 283	22.208	33.533	38.952	1.00 28.64	6
	ATOM	158	CG2		A 283	21.525	33.415	36.578	1.00 28.28	6
	ATOM	159	С		A 283	20.942	30.992	39.498	1.00 32.50	6
	ATOM	160	0	VAL .	A 283	21.879	30.717	40.229	1.00 33.48	8
	MOTA	161	N	VAL :	A 284	19.671	30.941	39.892	1.00 30.96	7
40	MOTA	162	CA	VAL	A 284	19.289	30.527	41.239	1.00 29.14	6
	MOTA	163	CB	VAL :	A 284	17.822	30.865	41.548	1.00 31.27	6
	MOTA	164	CG1	VAL 2	A 284	17.472	30.461	42.945	1.00 24.21	6
	MOTA	165	CG2	VAL	A 284	17.555	32.334	41.360	1.00 30.51	6
	MOTA	166	С	VAL	A 284	19.529	29.037	41.353	1.00 28.89	6
45	MOTA	167	0	VAL I	A 284	20.073	28.568	42.345	1.00 27.29	8
	ATOM	168	N	ASP Z	A 285	19.121	28.296	40.327	1.00 28.76	7
	ATOM	169	CA	ASP Z	A 285	19.277	26.842	40.306	1.00 35.32	6
	MOTA	170	CB	ASP 2	A 285	18.586	26.234	39.072	1.00 33.29	6
	ATOM	171	CG	ASP A	A 285	17.083	26.277	39.149	1.00 38.15	6
50	ATOM	172	OD1	ASP A	A 285	16.484	25.743	40.110	1.00 34.70	8
	ATOM	173	OD2	ASP A	A 285	16.431	26.828	38.231	1.00 34.43	8
	MOTA	174	С	ASP A	A 285	20.751	26.449	40.305	1.00 36.70	6
	ATOM	175	0	ASP Z	A 285	21.106	25.389	40.808	1.00 37.96	8
	MOTA	176	N	PHE A	A 286	21.604	27.300	39.737	1.00 35.96	7
55	ATOM	177	CA		A 286	23.029	27.022	39.704	1.00 37.10	6
	ATOM	178	CB		4 286	23.754	28.009	38.793	1.00 37.10	6
	MOTA	179	CG		4 286	25.252	28.027	38.987	1.00 36.50	6
	MOTA	180	CD1	PHE A		25.963	26.849	38.974	1.00 36.75	6
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5	ATOM	181	CD2	PHE A 286	25.931		39.199	1.00 33.83	6
•	ATOM	182	CEl	PHE A 286	27.331		39.161	1.00 39.55	6
	ATOM	183		PHE A 286	27.307		39.387	1.00 38.08	6
	ATOM	184		PHE A 286	28.008	28.052	39.371	1.00 34.44	6
	MOTA	185	C	PHE A 286	23.631	27.105	41.083	1.00 36.83	6
10	MOTA	186	0	PHE A 286	24.317	26.192	41.504	1.00 35.61	8
10	MOTA	187	N	ALA A 287	23.393	28.228	41.752	1.00 37.33	7
	MOTA	188	CA	ALA A 287	23.917	28.448	43.087	1.00 36.34	6
	ATOM	189	CB	ALA A 287	23.523	29.828	43.555	1.00 36.40	6
		190	C	ALA A 287	23.346	27.393	44.027	1.00 38.76	6
1 5	MOTA	191	0	ALA A 287	23.994	26.973	44.981	1.00 41.98	8
15	MOTA	192	И	LYS A 288	22.114	26.979	43.735	1.00 38.28	7
	ATOM	193	CA	LYS A 288	21.429	25.971	44.538	1.00 45.26	6
	MOTA	194	CB	LYS A 288	19.994	25.746	44.054	1.00 48.35	6
	MOTA	195	CG	LYS A 288	19.025	26.819	44.464	1.00 51.43	6
00	ATOM		CD	LYS A 288	17.628	26.246	44.682	1.00 60.23	6
20	MOTA	196	CE	LYS A 288	17.135	25.478	43.485	1.00 62.81	6
	MOTA	197		LYS A 288	17.196	26.327	42.268	1.00 64.69	7
	ATOM	198	NZ	LYS A 288	22.120	24.632	44.536	1.00 43.31	6
	MOTA	199	C	LYS A 288	21.967	23.857	45.462	1.00 45.66	8
~ ~	MOTA	200	0	LYS A 289	22.865	24.366	43.467	1.00 41.70	7
25	MOTA	201	N	LYS A 289	23.571	23.120	43.351	1.00 40.67	6
	MOTA	202	CA	LYS A 289	23.655	22.708	41.877	1.00 42.25	6
	ATOM	203	CB	LYS A 289	22.271	22.492	41.247	1.00 39.53	6
	MOTA	204	CG	LYS A 289	22.331	21.606	40.012	1.00 43.19	6
20	ATOM	205	CD	LYS A 289	20.941	21.362	39.447	1.00 45.74	6
30	MOTA	206	CE	LYS A 289	20.273	20.165	40.006	1.00 52.49	7
	MOTA	207	NZ	LYS A 289	24.948	23.185	44.003	1.00 41.50	6
	MOTA	208	С О	LYS A 289	25.642	22.184	44.080	1.00 39.77	8
	ATOM	209 210	N	LEU A 290	25.312	24.370	44.490	1.00 40.68	7
25	MOTA	211	CA	LEU A 290	26.594	24.583	45.149	1.00 39.33	6
35	MOTA	212	CB	LEU A 290	27.153	25.972	44.829	1.00 36.14	6
	MOTA	212	CG	LEU A 290	27.358	26.290	43.365	1.00 34.81	6
	ATOM	213	CD:		27.945	-	43.208	1.00 29.07	6
	ATOM	214			28.267		42.757	1.00 33.45	6
40	MOTA	215		LEU A 290	26.434		46.652		6
40	MOTA	217		LEU A 290	25.803		47.333	1.00 42.00	8
	MOTA	218		PRO A 291	27.028		47.210		7
	MOTA	219			27.851		46.519	1.00 39.65	6
•	ATOM	220			26.905			1.00 38.28	6
15	MOTA	221			27.755		48.911	1.00 35.88	6
45		222			28.202			1.00 34.19	6
	MOTA	223		PRO A 291	27.327			1.00 40.05	6
	ATOM	224		PRO A 291	26.571				8
	ATOM			MET A 292	28.522				7
50	ATOM	225			29.021				6
50		226			30.313				6
	MOTA	22			31.269				6
	ATOM	228			32.89				16
	ATOM	22			33.81				6
	MOTA	23							6
55		23		MET A 292	27.98				8
	MOTA	23		MET A 292	27.98				7
	MOTA	23		PHE A 293	27.08				6
	MOTA	23	4 C	A PHE A 293	26.03	0 28.091	47.11	1.00 40.02	•

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5	ATCM	235	CB	PHE	A	293	25.398	28.77	140 715	1.03	¥0.98	6
	ATCM	236	CG	PHE	A	293	24.348	29.168	47.524		42.78	6
	ATCM	237	CD1	PHE	A	293	24.654	30.493	47.747		44.40	6
	ATOM	238	CD2	PHE	A	293	23.071	28.833	47.116		43.66	6
	ATOM	239	CE1	PHE	A	293	23.701	31.478	47.564		39.83	6
10	ATCM	240	CE2	PHE	A	293	22.112	29.819	46.930		46.21	6
	ATOM	241	cz			293	22.430	31.146	47.155		45.18	6
	ATOM	242	С			293	24.979	27.772	50.164		45.54	
	ATOM	243	0			293	24.686	28.576	51.034		42.01	6
	ATOM	244	N	CYS			24.426	26.572	50.062		47.05	8
15	ATOM	245	CA	CYS		294	23.386	26.125	50.962		50.15	7
	ATOM	246	СВ	CYS		294	22.944	24.733	50.524		45.90	6
	ATOM	247	SG			294	22.303	24.663	48.829			6
	MOTA	248	C			294	23.825	26.125	52.423		51.50	16
	AŢOM	249	0			294	23.008	25.954			51.38	6
20	ATOM	250	N			295	25.119	26.327	53.322		53.83	8
	ATOM	251	CA			295	25.666	26.327	52.645		49.72	7
	ATOM	252	СВ			295	27.103	25.830	53.996		52.53	6
	ATOM	253	CG			295	27.103	•	54.015		57.40	6
	ATOM	254	CD			295	26.660	24.309	54.061		69.63	6
25	ATOM	255	OE1			295	27.291	23.747	55.342		78.49	6
	ATOM	256	OE2			295	25.590	23.946	56.412		82.82	8
	ATOM	257	C			295	25.653	23.086	55.335		85.30	8
	ATOM	258	0			295	26.365	27.831	54.488		48.54	6
	ATOM	259	N			296	24.804	28.184	55.426		49.82	8
30	ATOM	260	CA			296	24.670	28.631	53.846	1.00		7
	ATOM	261	CB			296	25.062	30.034	54.159	1.00		6
	MOTA	262	CG			296	26.438	30.864 30.658	52.923		41.04	6
	ATOM	263	CD1			296	26.447	31.030	52.315		42.74	6
	ATOM	264	CD2			296	27.437	31.454	50.861		40.99	6
35	ATOM	265	C			296	23.239	30.366	53.086	1.00	39.44	6
	ATOM	266	Ö			296	22.301	29.660	54.548		45.56	6
	ATOM	267	N			297	23.050	31.405	54.148 55.365		43.07	8
	ATOM	268	CD			297	24.121	32.241	55.930		46.99	7
	MOTA	269	CA	PRO			21.700	31.811	55.787		47.12	6
40	MOTA	270	СВ	PRO			21.937	32.990	56.738	1.00	49.61 49.91	6
	ATOM	271	CG	PRO			23.401	33.155	56.872			6
	ATOM	272	С	PRO			20.864	32.212	54.558		51.28 49.59	6
	ATOM	273	0	PRO			21.402	32.684	53.556		51.66	6
	ATOM	274	N	CYS			19.545	32.035	54.655		51.00	8
45	ATOM	275	CA	CYS			18.618	32.369	53.567		52.86	7
	ATOM	276	CB	CYS			17.201	31.877	53.915		54.57	6
	ATOM	277	SG	CYS			16.040	33.162	54.440		67.87	6
	MOTA	278	С	CYS			18.583	33.863	53.291		48.51	16
	MOTA	279	0	CYS			18.039	34.288	52.282			6
50	MOTA	280	N	GLU			19.144	34.654	54.202		49.58	8
	MOTA	281	CA	GLU			19.179	36.096	54.202		44.17	7
	MOTA	282	СВ	GLU			19.265	36.833	55.360		47.57	6
	MOTA	283	CG	GLU			17.931	36.996	56.125		49.92	6
	ATOM	284	CD	GLU			17.613	35.904	57.095		59.30	6
55	ATOM	285	OE1	GLU			16.512	35.952	57.706		63.80 69.03	6
	ATOM	286		GLU			18.436	34.976	57.706			8
	ATOM	287	С	GLU			20.359	36.492	53.152		67.10	8
	ATOM	288	0	GLU			20.265	37.441	52.379		46.57	6
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5 ATOM 289 N ASP A 300 21.467 35.76 293 3 30 1.00 43. ATOM 290 CA ASP A 300 22.661 36.042 52.509 1.00 43. ATOM 291 CB ASP A 300 23.919 35.513 53.213 1.00 37. ATOM 292 CG ASP A 300 24.223 36.239 54.473 1.00 36. ATOM 293 OD1 ASP A 300 24.153 37.488 54.493 1.00 35. ATOM 294 OD2 ASP A 300 24.572 35.575 55.483 1.00 40. ATOM 295 C ASP A 300 22.514 35.390 51.138 1.00 42. ATOM 296 O ASP A 300 22.775 36.021 50.113 1.00 46. ATOM 297 N GLN A 301 22.095 34.124 51.137 1.00 38. ATOM 298 CA GLN A 301 21.896 33.390 49.902 1.00 40. ATOM 299 CB GLN A 301 20.991 32.179 50.137 1.00 38. ATOM 300 CG GLN A 301 20.991 32.179 50.137 1.00 38. ATOM 301 CD GLN A 301 20.991 32.179 50.137 1.00 38. ATOM 302 OE1 GLN A 301 20.690 29.824 50.988 1.00 44. ATOM 303 NE2 GLN A 301 19.658 29.957 51.675 1.00 45. ATOM 303 NE2 GLN A 301 21.027 28.685 50.394 1.00 46. ATOM 304 C GLN A 301 21.242 34.305 48.877 1.00 41. ATOM 305 O GLN A 301 21.242 34.305 48.877 1.00 41.	7 7
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00E 0 0TN N 201 71 487 34.103 47.000 2.00 10	.02 8
ATOM 305 0 GLB R 302 20 413 35 228 49 372 1.00 41	.01 7
ATOM 306 N IEE A 302 10.726 36 179 48 511 1.00 40	.23 6
ATOM 307 CA 111 A 302 18 502 36 774 49 217 1.00 39	.52 6
ATOM 308 CB 112 A 300 17 818 37 788 48 342 1.00 31	.98 6
25 ATOM 309 CG2 IDE A 300 17 502 35 673 49 581 1.00 40	.77 6
ATOM 310 CG1 111 A 300 17 003 34 897 48 385 1.00 45	.43 6
ATOM 311 CD1 1D2 A 302 20 698 37 268 48.096 1.00 38	
ATOM 312 C IDE A 302 20.960 37.453 46.906 1.00 40	
ATOM 313 0 THE A 303 21.228 37.972 49.097 1.00 37	
30 AION 315 CD LLE D 303 22.179 39.060 48.874 1.00 39	.33 6
THOM 315 CR THE A 303 23.023 39.338 50.109 1.00 39	
NEOM 317 CG2 TLE A 303 23.946 40.522 49.861 1.00 36	
7 TON 318 CG1 TLE A 303 22.141 39.653 51.313 1.00 40	
35 ATOM 319 CD1 ILE A 303 22.916 39.806 52.589 1.00 30	
ATOM 320 C ILE A 303 23.093 38.705 47.722 1.00 30	
ATOM 321 O ILE A 303 23.354 39.509 46.835 1.00 3	
ATOM 322 N LEU A 304 23.580 37.477 47.762 1.00 3.	
ATOM 323 CA LEU A 304 24.465 36.964 46.734 1.00 2	
40 ATOM 324 CB LEU A 304 24.935 35.554 47.123 1.00 2	
ATOM 325 CG LEU A 304 26.150 35.480 48.029 1.00 2	
ATOM 326 CD1 LEU A 304 26.267 36.731 48.876 1.00 2	•
ATOM 327 CD2 LEU A 304 26.084 34.226 46.881 1.00 2	
ATOM 328 C LEU A 304 25.701 301 442 1 00 3	
45 ATOM 329 0 LEO A 304 24.222 310 1 00 3	
ATOM 330 N LEO A 303 22.037 30.22	
ATOM 331 CA LEO A 305 21.00 35 434 44 359 1 00 3	
ATOM 332 CB LEU A 303 200 037 33 050 44 635 1 00 3	
ATOM 333 CG LEU A 303 20.00, 00 and 1 00 a	
50 ATOM 334 CDI LEO A 303 13.240 23.280 43.466 1.00 3	
ATOM 335 CD2 LEG A 305 21 CC5 27 E24 43 477 1 00 2	
ATOM 336 C LEU A 335	
ATOM 337 0 EEU A 303 21.157 29 439 44 298 1 00 2	
ATOM 338 N LIS A 300 21.157 30.000 43.864 1.00	
55 ATOM 339 CA LIS A 500 200 40 615 45 026 1 00 1	
ATOM 340 CB EIS A 300 2010 40 163 45 511 1.00 4	
ATOM 341 CG LIS A 300 10.327 46 559 1 00 1	
ATOM 342 CD LYS A 306 18.397 41.127 46.559 1.00	

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5	ATOM	343		LYS A		18.271		•		
	ATOM	344		LYS A		18.325	43.548	47.038	1.00 59.61	7
	MOTA	345		LYS A		22.075	40.527	43.302	1.00 35.25	6
	MOTA	346		LYS A		21.972	41.286	42.334	1.00 33.95	8
	MOTA	347		GLY A		23.228	40.306	43.928	1.00 35.79	7 ·
10	MOTA	348		GLY A		24.445	40.962	43.482	1.00 34.59	6
	MOTA	349	С	GLY A	307	25.109	40.353	42.259	1.00 33.80	6
	MOTA	350	0	GLY A	307	25.489	41.087	41.344	1.00 31.59	8
	MOTA	351	N	CYS A	308	25.248	39.024	42.256	1.00 31.15	7
	MOTA	352	CA	CYS A	308	25.899	38.326	41.174	1.00 29.04	6
15	ATOM	353	CB	CYS A	308	26.604	37.089	41.704	1.00 27.59	6
	ATOM	354	SG	CYS A	308	25.472	35.770	42.071	1.00 30.50	16
	ATOM	355	С	CYS A	308	24.974	37.870	40.062	1.00 30.59	6
	MOTA	356	0	CYS A	308	25.458	37.319	39.077	1.00 33.77	8
	MOTA	357	N	CYS A	309	23.664	38.084	40.195	1.00 28.46	7
20	MOTA	358	CA	CYS A		22.739	37.623	39.168	1.00 30.10	6
	MOTA	359	СВ	CYS A		21.311	38.004	39.490	1.00 33.43	6
	MOTA	360	SG	CYS A	309	20.198	37.299	38.307	1.00 35.20	16
	ATOM	361	C	CYS A		23.065	38.123	37.788	1.00 27.72	6
	ATOM	362	ō	CYS A		23.212	37.334	36.865	1.00 27.69	8
25	MOTA	363	N	MET A		23.157	39.439	37.639	1.00 26.15	7
<i></i>	MOTA	364	CA	MET A		23.476	40.016	36.342	1.00 26.06	6
	MOTA	365	CB	MET A		23.482	41.547	36.419	1.00 25.32	6
	ATOM	366	CG	MET A		23.913	42.230	35.109	1.00 24.08	6
	ATOM	367	SD	MET A		22.765	41.751	33.762	1.00 27.71	16
30	ATOM	368	CE	MET A		23.650	42.321	32.270	1.00 28.50	6
50	ATOM	369	C	MET A		24.842	39.527	35.908	1.00 25.94	6
	MOTA	370	0	MET A		25.020	39.076	34.788	1.00 28.09	8
	ATOM	371	N	GLU A		25.800	39.638	36.826	1.00 25.39	7
	ATOM	372	CA	GLU A		27.176	39.234	36.589	1.00 27.03	6
35	MOTA	373	CB	GLU A		27.973	39.303	37.900	1.00 24.39	6
	ATOM	374	CG	GLU A		27.842	40.628	38.668	1.00 26.00	6
	ATOM	375	CD	GLU A		28.726	40.720	39.870	1.00 23.95	6
	MOTA	376	OE1	GLU A		28.891	39.706	40.588	1.00 19.72	8
	ATOM	377	OE2	GLU A		29.270	41.818	40.159	1.00 26.51	8
40	ATOM	378	C	GLU A		27.266	37.827	35.997	1.00 27.51	6
, ,	ATOM	379	0	GLU A		27.956	37.620	35.014	1.00 29.67	8
	MOTA	380	N	ILE A		26.569	36.866	36.602	1.00 26.82	7
	ATOM	381	CA	ILE A		26.593	35.497	36.112	1.00 25.71	6
	MOTA	382	CB	ILE A		25.991	34.518	37.123	1.00 23.35	6
45	ATOM	383		ILE A	312	25.917	33.123	36.533	1.00 20.27	6
	ATOM	384	CG1			26.837	34.471	38.398	1.00 20.88	6
	ATOM	385		ILE A		26.462	33.342	39.341	1.00 18.15	6
	ATOM	386		ILE A		25.871	35.371	34.791	1.00 27.91	6
	ATOM	387		ILE A		26.274	34.593	33.934	1.00 28.96	8
50	ATOM	388	N	MET A		24.788	36.130	34.633	1.00 27.66	7
20	ATOM	389		MET A		24.013	36.081	33.395	1.00 30.18	6
	ATOM	390		MET A		22.716	36.888	33.508	1.00 36.89	6
	ATOM	391		MET A		21.608	36.198	34.305	1.00 37.95	
	ATOM	392			313	19.892	36.817	34.055	1.00 42.38	
55	ATOM	393			A 313	20.034	38.503	34.740	1.00 40.68	
55	ATOM	394			313	24.834	36.579	32.222	1.00 27.43	
	ATOM	395			A 313	25.116	35.814	31.308	1.00 28.61	
	ATOM	396			A 314	25.209	37.859	32.253	1.00 24.88	
	ATOM	000	14	J 1						

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5	MOTA	397	CA	SER A		26.005	38.472	31.197	1.00 27.98	6
	ATOM	398	CB	SER A		26.354	39.914	31.581	1.00 29.64	6
	MOTA	399	OG	SER A	314	26.956	39.972	32.858	1.00 43.44	8
	MOTA	400	С	SER A	314	27.275	37.679	30.851	1.00 22.30	6
	MOTA	401	0	SER A	314	27.675	37.629	29.690	1.00 24.18	8
10	ATOM	402	N	LEU A	315	27.905	37.048	31.845	1.00 23.99	7
	MOTA	403	CA	LEU A	315	29.099	36.261	31.563	1.00 25.07	6
	MOTA	404	CB	LEU A	315	29.685	35.593	32.816	1.00 19.11	6
	ATOM	405	CG	LEU A		30.675	34.479	32.505	1.00 20.39	6
	ATOM	406	CD1	LEU A		31.866	35.040	31.756	1.00 18.92	6
15	ATOM	407	CD2	LEU A		31.125	33.789	33.765	1.00 12.93	6
	ATOM	408	C	LEU A		28.700	35.180	30.597	1.00 24.53	6
	ATOM	409	0	LEU A		29.304	35.036	29.556	1.00 24.33	8
•	ATOM	410	N	ARG A		27.678	34.426	30.982	1.00 28.18	7
	ATOM	411	CA	ARG A		27.151	33.312	30.216	1.00 20.18	6
20				ARG A		25.915	32.752	30.210	1.00 27.34	6
20	ATOM	412	CB	ARG A						
	ATOM	413	CG			26.188	32.190	32.336	1.00 22.00	6
	ATOM	414	CD	ARG A		24.934	31.526	32.901	1.00 18.78	6
	MOTA	415	NE	ARG A		25.245	30.376	33.721	1.00 26.57	7
0.5	MOTA	416	CZ	ARG F		24.341	29.468	34.054	1.00 30.81	6
25	MOTA	417	NH1	ARG F		23.084	29.614	33.639	1.00 33.71	7
	ATOM	418		ARG F		24.701	28.416	34.776	1.00 33.13	7
	ATOM	419	С	ARG A		26.774	33.660	28.794	1.00 28.09	6
	ATOM	420	0	ARG F		26.737	32.792	27.931	1.00 32.41	8
	MOTA	421	N	ALA A		26.484	34.936	28.571	1.00 28.36	7
30	MOTA	422	CA	ALA A		26.094	35.411	27.264	1.00 26.64	6
	MOTA	423	CB	ALA A		25.232	36.666	27.418	1.00 22.93	6
	MOTA	424	C	ALA A		27.323	35.714	26.417	1.00 28.35	6
	MOTA	425	0	ALA A		27.398	35.342	25.252	1.00 32.10	8
	ATOM	426	N	ALA A		28.286	36.396	27.026	1.00 29.12	7
35	ATOM	427	CA	ALA A		29.515	36.760	26.350	1.00 27.50	6
	MOTA	428	CB	ALA A		30.434	37.452	27.333	1.00 28.39	6
	MOTA	429	С	ALA A		30.181	35.502	25.825	1.00 28.10	6
	MOTA	430	0	ALA A		30.600	35.447	24.678	1.00 28.18	8
	MOTA	431	N	VAL A		30.255	34.491	26.700	1.00 29.16	7
40	ATOM	432	CA	VAL A		30.880	33.198	26.393	1.00 35.24	6
	MOTA	433	CB	VAL A		30.703	32.210	27.547	1.00 27.34	6
	ATOM	434	CG1	VAL A		30.895	32.891	28.858	1.00 29.96	6
	ATOM	435		VAL A		29.353	31.552	27.482	1.00 31.70	6
	MOTA	436	С	VAL A		30.215	32.608	25.165	1.00 40.01	6
45	MOTA	437	0	VAL A		30.640	31.575	24.680	1.00 42.70	8
	MOTA	438	N	ARG A		29.176	33.284	24.683	1.00 38.64	7
	MOTA	439	CA	ARG A	320	28.415	32.822	23.545	1.00 38.61	6
	ATOM	440	CB	ARG A		27.031	32.458	24.043	1.00 37.26	6
	ATOM	441	CG	ARG A	320	26.863	30.991	24.192	1.00 43.12	6
50	MOTA	442	CD	ARG A	320	25.637	30.642	25.014	1.00 50.79	6
	ATOM	443	NE	ARG A	320	25.258	29.256	24.770	1.00 54.71	7
	MOTA	444	CZ	ARG A		24.331	28.625	25.501	1.00 57.89	6
	ATOM	445	NH1	ARG A	320	23.667	29.291	26.440	1.00 49.08	7
	ATOM	446		ARG A		23.964	27.385	25.242	1.00 59.59	7
55	ATOM	447	С	ARG A		28.292	33.825	22.405	1.00 42.14	6
	ATOM	448	0	ARG A		27.251	33.909	21.748	1.00 46.30	8
	ATOM	449	N	TYR A		29.352	34.583	22.173	1.00 42.04	7
	ATOM	450	CA	TYR I		29.366	35.555	21.098	1.00 42.70	6
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5	ATOM	451		YR A		30.0		36.810	21.5			38.01	6
	ATOM	452		TYR A		30.6		37.650	20.4			37.94	6
	MOTA	453	CD1 7	ryr A	321	29.7		38.296	19.5			33.85	6
	MOTA	454		ryr A		30.2		39.037	18.4			34.49	6
	MOTA	455		ryr A		31.9		37.743	20.2			28.03	6
10	MOTA	456	CE2	ryr A	321	32.4		38.475	19.1			32.69	6
	MOTA	457	CZ :	TYR A	321	31.6	12	39.125	18.2			35.18	6
	ATOM	458	OH '	ryr A	321	32.1		39.866	17.2			39.48	8
	ATOM	459	C	TYR A	321	30.0	85	35.005	19.8			45.51	6
	MOTA	460	0 '	TYR A	321	31.2		34.697	19.9			48.02	8
15	MOTA	461	N .	ASP A	322	29.3		34.879	18.7			44.56	7
	ATOM	462	CA	ASP A	322	29.9		34.400	17.5			45.86	6
	MOTA	463	CB :	ASP A	322 ·	28.8	304	33.670	16.7			46.64	6
	MOTA	464	CG .	ASP A	322	29.0	50	33.608	15.2			40.00	6
	MOTA	465	OD1	ASP A	322	30.0	010	34.256	14.7			40.00	8
20	MOTA	466	OD2	ASP A	322	28.2	262	32.929	14.5			40.00	8
	ATOM	467	С	ASP A	322	30.	460	35.629	16.	755		45.82	6
	ATOM	468		ASP A	322	29.	678	36.464	16.2	271		45.38	8
	MOTA	469	N	PRO A	323	31.	800	35.735	16.	584	1.00	46.53	7
	MOTA	470	CD	PRO A	323	32.	774	34.719	16.	991		47.16	6
25	MOTA	471	CA	PRO A	323	32.	424	36.889	15.	890		46.63	6
	ATOM	472	CB	PRO A	323	33.	921	36.603	15.	936		43.95	6
	MOTA	473	CG	PRO A	323	34.	099	35.303	16.	582		43.93	6
	ATOM	474	С	PRO A	323	31.	953	37.087	14.	453		48.34	6
	MOTA	475	0	PRO A	323	31.	797	38.210	13.	960		50.84	8
30	MOTA	476	N	GLU A	324	31.	778	35.970	13.	752		52.39	7
	ATOM	477	CA	GLU A	324	31.	339	35.968	12.	370		55.85	6
	MOTA	478	CB	GLU A	324	31.	035	34.528	11.			55.54	6
	MOTA	479	CG	GLU A	324	32.	224	33.584	12.			40.00	6
	MOTA	480	CD	GLU A	324	33.	432	34.023	11.			40.00	6
35	MOTA	481	OE1	GLU A	324		350	35.040	10.			40.00	8
	MOTA	482	OE2	GLU A		34.	506	33.356		415		40.00	8
	MOTA	483	С	GLU A			077	36.798		277		54.94	6
	MOTA	484	0	GLU A			070	37.892		730	1.00		8
	MOTA	485	N	SER A			009	36.212		810		52.95	7
40	MOTA	486	CA	SER A			695	36.812		839		50.10	6
	ATOM	487	CB	SER A			701	35.797		402		48.23	6
	MOTA	488	OG	SER A			183	35.239				48.71	8
	MOTA	489	С	SER A			651	38.093		659		50.61	6
	MOTA	490	0	SER A			885	38.992		354		52.19	8
45	MOTA	491	N	GLU A			495	38.168		687		45.64	7
	MOTA	492	CA	GLU A			567	39.341		546		43.35	6
	MOTA	493	CB	GLU A			830	40.608		711		42.74	6
	MOTA	494	CG	GLU F			148	40.606		945		50.32	6
	ATOM	495		GLU F			451	41.925		313		56.34	6
50	MOTA	496		GLU F			.509	42.046		649		59.31	8
	ATOM	497					656	42.890		452		55.74	8
	ATOM	498		GLU F			.288	39.526		340		40.23	6
	MOTA	499		GLU A			. 695	40.603		340		40.44	8
	MOTA	500		THR A			.888	38.474		.051		35.90	7
55	MOTA	501		THR A			. 663	38.506		.860		37.29	6
	MOTA	502		THR A			. 466	38.057		.024		37.63	6
	MOTA	503					.661	36.709		.580		38.12	8
	ATOM	504	CG2	THR A	A 327	24	.269	38.965	15.	.810	1.00	39.90	6

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5	ATOM	505	С	THR A	327	25.767	37.562	19.038	1.00 39.49	б
	MOTA	506	0	THR A	327	26.284	36.458	18.903	1.00 40.50	8
	ATOM	507	N	LEU A	328	25.250	37.987	20.184	1.00 36.64	7
	ATOM	508	CA	LEU A	328	25.264	37.141	21.381	1.00 37.73	6
	MOTA	509	CB	LEU A	328	25.148	37.999	22.650	1.00 37.78	6
10	ATOM	510	CG	LEU A	328	26.102	39.150	22.843	1.00 36.26	6
	MOTA	511	CD1	LEU A	328	26.066	39.623	24.272	1.00 36.56	6
	ATOM	512	CD2	LEU A	328	27.481	38.688	22.500	1.00 39.85	6
	ATOM	513	С	LEU A	328	24.063	36.220	21.244	1.00 37.27	6
	MOTA	514	0	LEU A	328	23.306	36.337	20.279	1.00 34.96	8
15	MOTA	515	N	THR A	329	23.891	35.317	22.205	1.00 39.73	7
	ATOM	516	CA	THR A	329	22.785	34.376	22.180	1.00 40.81	6
	ATOM	517	CB	THR A	329	23.241	32.991	21.699	1.00 42.67	6
	MOTA	518	OG1	THR A		23.879	33.103	20.421	1.00 42.52	8
	ATOM	519	CG2	THR A		22.026	32.057	21.589	1.00 43.52	6
20	ATOM	520	С	THR A		22.168	34.245	23.548	1.00 44.31	6
	ATOM	521	0	THR A		22.526	33.370	24.320	1.00 43.72	8
	ATOM	522	N	LEU P		21.237	35.149	23.830	1.00 44.62	7
	MOTA	523	CA	LEU A		20.532	35.170	25.111	1.00 45.09	6
	ATOM	524	СВ	LEU F		19.677	36.444	25.195	1.00 44.66	6
25	ATOM	525	CG	LEU A		20.436	37.750	25.259	1.00 51.06	6
	ATOM	526	CD1	LEU F		21.405	37.831	24.104	1.00 48.58	6
	ATOM	527	CD2	LEU A		19.466	38.909	25.238	1.00 45.18	6
	ATOM	528	С	LEU A		19.656	33.919	25.301	1.00 48.06	6
	ATOM	529	0	LEU A		19.049	33.422	24.359	1.00 49.33	8
30	ATOM	530	N	ASN A		19.618	33.431	26.540	1.00 52.20	7
	MOTA	531	CA	ASN A		18.842	32.256	26.913	1.00 54.41	6
	ATOM	532	СВ	ASN A		17.361	32.628	27.009	1.00 54.94	6
	ATOM	533	CG	ASN A		16.724	32.112	28.269	1.00 60.35	6
	MOTA	534	OD1	ASN A		17.124	32.505	29.383	1.00 61.84	8
35	MOTA	535	ND2	ASN A		15.750	31.238	28.117	1.00 65.92	7
	MOTA	536	С	ASN A	331	19.016	31.108	25.934	1.00 58.00	6
	MOTA	537	0	ASN A	331	18.243	30.157	25.941	1.00 60.17	8
	ATOM	538	N	GLY A	332	20.063	31.196	25.114	1.00 58.45	7
	MOTA	539	CA	GLY A	332	20.341	30.161	24.131	1.00 58.55	6
40	MOTA	540	С	GLY A	A 332	19.316	30.016	23.021	1.00 59.79	6
	MOTA	541	0	GLY Z	A 332	19.413	29.094	22.213	1.00 61.32	8
	ATOM	542	N	GLU A	A 333	18.346	30.929	22.983	1.00 60.28	7
	MOTA	543	CA	GLU 2	333	17.294	30.883	21.985	1.00 59.13	6
	MOTA	544	CB	GLU Z	8 333	15.919	30.875	22.662	1.00 62.40	6
45	ATOM	545	CG	GLU 2	A 333	15.667	29.750	23.658	1.00 75.69	6
	MOTA	546	CD	GLU A	8 333	14.341	29.865	24.346	1.00 80.41	6
	ATOM	547	OE1	GLU Z	8 3 3 A	14.052	30.932	24.945	1.00 79.98	8
	ATOM	548	OE2	GLU 2	A 333	13.549	28.884	24.329	1.00 83.81	8
	MOTA	549	С	GLU	8 333	17.356	32.090	21.073	1.00 57.18	6
50	MOTA	550	0	GLU 2	8 333	17.239	31.969	19.852	1.00 57.50	8
	MOTA	551	N	MET	A 334	17.512	33.258	21.696	1.00 55.20	7
	MOTA	552	CA	MET .	A 334	17.561	34.529	20.980	1.00 50.85	6
	ATOM	553	СВ	MET .	A 334	16.751	35.556	21.763	1.00 48.70	6
	MOTA	554	CG	MET .	A 334	16.859	36.947	21.212	1.00 45.39	6
55	ATOM	555	SD	MET .	A 334	15.881	38.186	22.127	1.00 44.56	16
	MOTA	556	CE	MET :	A 334	14.229	37.371	22.113	1.00 45.25	6
	MOTA	557	С	MET .	A 334	18.956	35.087	20.713	1.00 51.59	6
	ATOM	558	0	MET .	A 334	19.739	35.268	21.633	1.00 52.52	8

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5	ATOM	559	N	ALA	A	335	19.234	35.371	19.444	1.00	51.00	7
	ATOM	560	CA			335	20.520	35.932	19.039		48.98	6
	ATOM	561	СВ			335	20.997	35.254	17.768		47.86	6
	ATOM	562	С			335	20.342	37.420	18.805		51.01	
	ATOM	563	Ō			335	19.594	37.420	17.919			6
10	ATOM	564	N			336	21.024				51.61	8
	ATOM	565	CA			336		38.232	19.612		46.62	7
	ATOM	566					20.910	39.699	19.502		42.35	6
			CB			336	20.517	40.325	20.840		42.41	6
	MOTA	567	CG1			336	19.242	39.691	21.361	1.00		6
15	MOTA	568	CG2			336	21.639	40.211	21.852		40.32	6
15	ATOM	569	С			336	22.204	40.321	19.036	1.00	45.33	6
	MOTA	570	0			336	23.263	39.691	19.025	1.00	47.42	8
	MOTA	571	И	THR	Α	337	22.090	41.590	18.668	1.00	41.60	7
	ATOM	572	CA	THR	Α	337	23.230	42.377	18.175	1.00	39.69	6
	ATOM	573	CB	THR	A	337	22.882	43.061	16.852		41.35	6
20	MOTA	574	OG1	THR	Α	337	21.987	44.157	17.080		49.35	8
	ATOM	575	CG2	THR	Α	337	22.216	42.067	15.904		40.38	6
	ATOM	576	С	THR	Α	337	23.588	43.481	19.159		37.88	6
	MOTA	577	0			337	22.734	43.989	19.892		34.06	8
	MOTA	578	N			338	24.865	43.849	19.138		37.61	7
25	MOTA	579	CA			338	25.388	44.919	19.984		38.68	6
	ATOM	580	СВ			338	26.669	45.479	19.351		35.95	
	ATOM	581	CG			338	27.250	46.713	20.038			6
	MOTA	582	CD			338	28.443	47.254			38.83	6
	ATOM	583	NE			338	29.559	46.320	19.247		35.88	6
30	ATOM	584	CZ			338	30.449		19.175		37.42	7
	ATOM	585	NH1			338		46.122	20.145		30.20	6
	MOTA	586	NH2			338	30.338	46.791	21.295		27.98	7
	ATOM	587	C			338	31.433	45.240	19.954		27.40	7
	MOTA	588	0			338	24.333	46.010	20.085		38.09	6
35	MOTA	589	N				23.894	46.397	21.169		34.12	8
"	MOTA	590				339	23.915	46.496	18.922		41.25	7
			CA			339	22.918	47.547	18.890		41.35	6
	ATOM	591	С			339	21.692	47.140	19.672		41.23	6
	ATOM	592	0			339	21.445	47.671	20.750		38.30	8
40	ATOM	593	N			340	20.924	46.203	19.105		38.58	7
40	ATOM	594	CA			340	19.701	45.700	19.729			6
	ATOM	595	CB			340	19.436	44.260	19.253		40.82	6
	ATOM	596	CG			340	19.087	44.146	17.767	1.00	41.10	6
	ATOM	.597	CD			340	18.876	42.705	17.305	1.00	48.84	6
4.5	ATOM	598		GLN			19.826	41.888	17.309	1.00	50.53	8
45	ATOM	599		GLN			17.650	42.393	16.907	1.00	54.25	7
	MOTA	600	С			340	19.779	45.750	21.263	1.00	41.50	6
	MOTA	601	0	GLN	Α	340	18.998	46.444	21.923	1.00	42.72	8
	ATOM	602	N	LEU	A	341	20.758	45.026	21.806	1.00	42.00	7
	MOTA	603	CA	LEU	Α	341	20.952	44.947	23.243		38.10	6
50	MOTA	604	CB	LEU	Α	341	22.209	44.145	23.575		36.66	6
	ATOM	605	CG	LEU	Α	341	22.361	43.804	25.029		39.94	6
	ATOM	606	CD1	LEU	A	341	21.219	42.884	25.410		34.98	6
	MOTA	607		LEU			23.685	43.128	25.284		40.95	6
	MOTA	608	С	LEU			21.072	46.321	23.860		36.37	6
55	ATOM	609	0	LEU			20.484	46.588	24.892		37.89	8
	MOTA	610	N	LYS			21.848	47.184	23.209		33.29	7
	ATOM	611	CA	LYS			22.089	48.546	23.209		35.29 35.17	
	ATOM	612	CB	LYS			23.057					6
		V + 4	22		47	J32	23.03/	49.242	22.721	1.00	34.9/	6

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	W O 33/000	0014		5
5	ATOM	613 CG LYS A 342	23.655 50.536 23.240 1.00 40.00	6 ° 🤋
,	ATOM	614 CD LYS A 342	24.673 51.109 22.245 1.00 34.48	6
	MOTA	615 CE LYS A 342	25.514 52.229 22.873 1.00 37.54	6
	MOTA	616 NZ LYS A 342	26.655 52.634 21.987 1.00 42.32	7
	ATOM	617 C LYS A 342	20.796 49.349 23.774 1.00 38.29	8
10	MOTA	618 O LYS A 342	20.345 49.711 24.861 1.00 36.23	8
10	ATOM	619 N ASN A 343	20.223 49.622 22.603 1.00 39.25	7
	ATOM	620 CA ASN A 343	18.993 50.385 22.485 1.00 40.19	6
	MOTA	621 CB ASN A 343	18.521 50.373 21.033 1.00 37.96	6
	ATOM	622 CG ASN A 343	19.664 50.550 20.052 1.00 39.22	6
15	ATOM	623 OD1 ASN A 343	20.428 51.537 20.125 1.00 42.37	8
13	MOTA	624 ND2 ASN A 343	19.773 49.612 19.125 1.00 42.19	7
	ATOM	625 C ASN A 343	17.928 49.748 23.375 1.00 40.12	6
	MOTA	626 O ASN A 343	17.010 50.417 23.859 1.00 36.01	8
	ATOM	627 N GLY A 344	18.073 48.433 23.568 1.00 40.95	7
20	MOTA	628 CA GLY A 344	17.152 47.670 24.394 1.00 39.25	6
20	ATOM	629 C GLY A 344	17.039 48.092 25.842 1.00 38.26	6
	ATOM	630 O GLY A 344	16.072 47.724 26.512 1.00 35.69	8
	MOTA	631 N GLY A 345	18.017 48.857 26.329 1.00 35.89	7
	MOTA	632 CA GLY A 345	17.964 49.301 27.706 1.00 34.00	6
25	ATOM	633 C GLY A 345	19.273 49.199 28.443 1.00 38.64	6
23	ATOM	634 O GLY A 345	19.469 49.888 29.441 1.00 38.14	8
	MOTA	635 N LEU A 346	20.170 48.337 27.973 1.00 39.52	7
	ATOM	636 CA LEU A 346	21.444 48.180 28.649 1.00 36.05	6
	MOTA	637 CB LEU A 346	22.124 46.876 28.209 1.00 35.72	6
30	MOTA	638 CG LEU A 346	21.355 45.617 28.501 1.00 34.89	6
30	ATOM	639 CD1 LEU A 346	22.295 44.413 28.422 1.00 44.09	6
	ATOM	640 CD2 LEU A 346	20.786 45.721 29.902 1.00 34.84	6
	MOTA	641 C LEU A 346	22.358 49.361 28.396 1.00 33.52	6
	ATOM	642 O LEU A 346	23.267 49.653 29.178 1.00 35.58	8
35	ATOM	643 N GLY A 347	22.087 50.056 27.295 1.00 30.47	7 .
50	ATOM	644 CA GLY A 347	22.909 51.192 26.931 1.00 33.01	6
	ATOM	645 C GLY A 347	24.360 50.768 26.747 1.00 30.72	6
	ATOM	646 O GLY A 347	24.669 49.775 26.082 1.00 30.89	8
	MOTA	647 N VAL A 348	25.244 51.556 27.355 1.00 31.30	7
40	ATOM	648 CA VAL A 348	26.671 51.325 27.286 1.00 31.27	6
	MOTA	649 CB VAL A 348	27.441 52.294 28.184 1.00 31.66	6
	MOTA	650 CG1 VAL A 348	27.067 52.107 29.631 1.00 20.19	6
	ATOM	651 CG2 VAL A 348	28.931 52.138 27.986 1.00 24.77	6
	ATOM	652 C VAL A 348	27.063 49.892 27.678 1.00 33.84	6
45	ATOM	653 O VAL A 348	28.095 49.392 27.225 1.00 29.99	8
	ATOM	654 N VAL A 349	26.253 49.227 28.514 1.00 33.31	7
	ATOM	655 CA VAL A 349	26.568 47.881 28.906 1.00 32.23	6
	MOTA	656 CB VAL A 349	25.581 47.259 29.858 1.00 32.59	
	ATOM	657 CG1 VAL A 349	25.865 45.795 29.985 1.00 33.68	6
50	MOTA	658 CG2 VAL A 349	25.687 47.899 31.213 1.00 32.30	
	MOTA	659 C VAL A 349	26.706 46.985 27.726 1.00 34.91	6
	ATOM	660 O VAL A 349	27.583 46.136 27.735 1.00 33.73	8
	ATOM	661 N SER A 350	25.875 47.134 26.702 1.00 32.81	
	ATOM	662 CA SER A 350	26.001 46.252 25.556 1.00 30.10	
55		663 CB SER A 350	25.119 46.665 24.411 1.00 24.95	
	MOTA	664 OG SER A 350	25.209 45.675 23.394 1.00 23.16	
	MOTA	665 C SER A 350	27.445 46.257 25.129 1.00 31.59	
	MOTA	666 O SER A 350	28.116 45.244 25.284 1.00 37.62	8

5	MOTA	667	N	ASP A	351	27.945	47.364	6 591	1.00 28.60	7
	ATOM	668	CA	ASP A	351	29.351	47.437	24.183	1.00 29.82	6
	MOTA	669	СВ	ASP A		29.808	48.891	24.105	1.00 27.49	6
	MOTA	670	CG	ASP A	351	28.875	49.744	23.303	1.00 30.22	6
	MOTA	671	OD1	ASP A		28.055	50.483	23.909	1.00 32.61	8
10	ATOM	672	OD2	ASP A	351	28.942	49.714	22.044	1.00 30.02	8
	MOTA	673	С	ASP A	351	30.173	46.653	25.231	1.00 30.63	6
	MOTA	674	0	ASP A	351	30.981	45.792	24.903	1.00 29.54	8
	MOTA	675	N	ALA A		29.939	46.949	26.503	1.00 25.33	7
	MOTA	676	CA	ALA A		30.623	46.280	27.602	1.00 28.59	6
15	ATOM	677	CB	ALA A		30.072	46.799	28.922	1.00 20.95	6
	ATOM	678	С	ALA A		30.492	44.756	27.527	1.00 29.69	6
	ATOM	679	0	ALA A		31.481	44.054	27.587	1.00 30.36	8
	MOTA	680	N	ILE A		29.260	44.260	27.413	1.00 27.63	7
	ATOM	681	CA	ILE A		29.003	42.832	27.326	1.00 27.55	6
20	ATOM	682	СВ	ILE A		27.512	42.528	27.429	1.00 28.04	6
	ATOM	683	CG2	ILE A		27.269	41.042	27.289	1.00 23.68	6
	ATOM	684	CG1	ILE A		26.955	42.965	28.789	1.00 27.33	6
	ATOM	685	CD1	ILE A		25.452	42.688	28.944	1.00 26.23	6
	ATOM	686	С	ILE A		29.534	42.207	26.054	1.00 30.88	6
25	ATOM	687	Ō	ILE A		30.007	41.076	26.068	1.00 30.00	8
	ATOM	688	N	PHE A		29.426	42.917	24.939	1.00 31.22	7
	ATOM	689	CA	PHE A		29.922	42.369	23.686	1.00 23.00	6
	MOTA	690	CB	PHE A		29.371	43.146	22.487	1.00 28.80	6
	ATOM	691	CG	PHE A		28.029	42.643	21.988	1.00 28.80	6
30	ATOM	692	CD1	PHE A		26.872	42.842	22.724	1.00 30.96	6
	ATOM	693	CD2	PHE A		27.950	41.953	20.783	1.00 30.30	6
	MOTA	694	CE1	PHE A		25.657	42.360	22.250	1.00 27.12	6
	ATOM	695	CE2	PHE A		26.738	41.470	20.305	1.00 25.19	6
	MOTA	696	CZ	PHE A		25.590	41.672	21.038	1.00 28.09	6
35	ATOM	697	C	PHE A		31.444	42.399	23.682	1.00 29.17	6
	ATOM	698	0	PHE A		32.087	41.389	23.398	1.00 32.62	8
	MOTA	699	N	ASP A		32.013	43.569	23.980	1.00 23.86	7
	ATOM	700	CA	ASP A		33.466	43.739	24.030	1.00 25.34	6
	ATOM	701	CB	ASP A		33.820	45.053	24.737	1.00 21.41	6
40	ATOM	702	CG	ASP A		33.841	46.226	23.809	1.00 32.08	6
	ATOM	703	OD1	ASP A		32.979	46.322	22.902	1.00 33.58	8
	ATOM	704	OD2	ASP A	355	34.711	47.117	23.968	1.00 33.20	8
	ATOM	705	С	ASP A		34.074	42.559	24.781	1.00 27.86	6
	ATOM	706	0	ASP A	355	35.131	42.053	24.410	1.00 32.42	8
45	MOTA	707	N	LEU A	356	33.387	42.128	25.843	1.00 26.84	7
	ATOM	708	CA	LEU A		33.845	40.993	26.642	1.00 28.66	6
	ATOM	709	СВ	LEU A		32.893	40.747	27.825	1.00 25.37	6
	ATOM	710	CG	LEU A		33.235	39.608	28.755	1.00 27.61	6
	MOTA	711	CD1	LEU A		34.538	39.917	29.451	1.00 25.43	6
50	ATOM	712	CD2	LEU A		32.149	39.414	29.765	1.00 27.49	6
	ATOM	713	С	LEU A		33.849	39.779	25.723	1.00 30.44	6
	ATOM	714	0	LEU A		34.884	39.160	25.470	1.00 31.55	8
	ATOM	715	N	GLY A		32.661	39.451	25.218	1.00 32.69	7
	ATOM	716	CA	GLY A		32.511	38.304	24.338	1.00 32.09	6
55	ATOM	717	C	GLY A		33.653	38.157	23.359	1.00 23.87	6
	ATOM	718	Ō	GLY A		34.302	37.110	23.323	1.00 33.12	8
	ATOM	719	N	MET A		33.876	39.206	22.564	1.00 29.41	7
	ATOM	720	CA	MET A		34.949	39.206	21.580	1.00 35.31	6
			- · -				33.200		4.00 33.07	J

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5	ATCM	721 CB				40.6				6 6
_	ATOM	722 CG	MET A 3	58			20.290	1.00 4		
	ATOM	723 SD	MET A 3	58	34.207		19.514	1.00 4		16
	ATOM	724 CE	MET A 3	58	34.507		20.994		4.29	6
	ATOM	725 C	MET A 3		36.256		22.230	1.00 3		6
10	ATOM	726 0	MET A 3		36.894	37.807	21.795	1.00 3		8
10	ATOM	727 N	SER A 3		36.637	39.491	23.281		33.31	7
	ATOM	728 CF			37.860	39.226	24.019		34.39	6
	ATOM	729 CE			37.869	40.067	25.295		30.84	6
	ATOM	730 00	_		39.135	40.008	25.930	1.00		8
15	ATOM	731 C	SER A 3		37.984	37.748	24.357		36.43	6
13	ATOM	732 0	SER A 3		38.900	37.078	23.896	1.00		8
	ATOM	732 N	_		37.046	37.264	25.166	1.00		7
		734 C			37.017	35.875	25.604	1.00	35.44	6
	ATOM	734 C			35.708	35.579	26.336	1.00		6
20	ATOM	736 C			35.471	36.290	27.644	1.00	34.59	6
20	ATOM		D1 LEU A		34.225	35.765	28.312	1.00	33.53	6
	MOTA		D2 LEU A		36.658	36.052	28.541	1.00	31.69	6
	ATOM				37.203	34.862	24.500	1.00	38.72	6
	ATOM	739 C			37.820	33.828	24.728	1.00	38.29	8
~~	ATOM	740 0			36.635	35.147	23.328	1.00	40.96	7
25	MOTA	741 N			36.777	34.262	22.186	1.00	45.67	6
	MOTA				36.518	35.045	20.904	1.00	46.45	6
	ATOM				35.210	35.598	20.906	1.00	51.81	8
	MOTA				38.166	33.627	22.145	1.00	44.49	6
	MOTA	745			38.347	32.538	21.625	1.00	46.67	8
30	ATOM	746			39.134	34.348	22.703		41.44	7
	MOTA	747 N			40.525	33.918	22.790	1.00	42.13	6
	MOTA				41.408	35.131	23.066	1.00	42.61	6
	MOTA				41.219	36.136	22.076	1.00	51.87	8
	ATOM				40.798	32.870	23.876	1.00	38.41	6
35	MOTA				41.553	31.938	23.641	1.00	38.01	8
	MOTA				40.198	33.039	25.058	1.00	34.55	7
	MOTA				40.417	32.126	26.174	1.00	32.96	6
	MOTA				39.832	32.718	27.447	1.00	31.99	6
40	MOTA				40.448	34.036	27.840	1.00	29.97	6
40	ATOM		CG PHE A		40.102	34.650	29.020	1.00	30.61	6
	MOTA		CD1 PHE A		41.379				32.02	6
	MOTA		CE1 PHE A		40.685		29.391		33.67	6
	MOTA		CE2 PHE A		41.959				30.91	6
	MOTA				41.615				29.33	6
45					39.883				30.52	
	MOTA	762	C PHE A		40.436				32.19	
	MOTA	763	O PHE A		38.817				33.51	
	MOTA	764	N ASN A		38.239				38.03	
	ATOM	765	CA ASN A		39.240				42.32	
50		766	CB ASN A		39.240				53.11	
	ATOM	767	CG ASN A						59.51	
	MOTA	768	OD1 ASN A		38.874				55.95	
	MOTA	769	ND2 ASN A		40.986	_			31.89	
	MOTA	770	C ASN A		37.916				30.28	
55	MOTA	771	O ASN A		38.324				27.62	
	MOTA	772	N LEU A		37.176				29.36	
	MOTA	773	CA LEU P		36.806				27.54	
	MOTA	774	CB LEU F	365	36.195	29.866	29.43	, 1.00	, <u> </u>	_

			26 990 31 150 29.185 1.00 38.91 6
5	MOTA	775 CG LEU A 365	30.990 31.130 30.34 47 6
•	ATOM	776 CD1 LEU A 365	30.316 32.210
	MOTA	777 CD2 LEU A 365	30.400 30.003 20.000 1 00 26 23 6
	MOTA	778 C LEU A 365	35.630 27.390 20.00
	ATOM	779 O LEU A 365	34.690 27.049 2.111
10	MOTA	780 N ASP A 366	36.083 26.320 23.000
	MOTA	781 CA ASP A 366	35.213 25.330 20.00 1 00 00 60
	MOTA	782 CB ASP A 366	30.027 23.030
	ATOM	783 CG ASP A 366	36.799 23.074 30.000 1.00 26.70
	MOTA	784 OD1 ASP A 366	36.265 24.177 31.33
15	MOTA	785 OD2 ASP A 366	37.959 25.500 55.201 1.00 27.70
	ATOM	786 C ASP A 366	34.270 25.454 35.450 1.00 31.04
	MOTA	787 O ASP A 366	34.307 20.000 1 00 20 10 7
	MOTA	788 N ASP A 367	33.111 211111 2 100 7 00 77 77 6
	ATOM	789 CA ASP A 367	32.120 24.073 32.123
20	MOTA	790 CB ASP A 367	31.472 23.201
20	ATOM	791 CG ASP A 367	50.000
	ATOM	792 OD1 ASP A 367	29.877 23.000 20.000 1.00 51.42
	MOTA	793 OD2 ASP A 367	31.100 21.004 23.00
	ATOM	794 C ASP A 367	32.734 24.909 02.00
25	MOTA	795 O ASP A 367	32.464 20.000 33.000
23	ATOM	796 N THR A 368	33.602 24.032 32.323
	MOTA	797 CA THR A 368	34.329 24.124 34.114 1 00 07 30 6
	MOTA	798 CB THR A 368	35.559 23.222 37.222 1.00.23.42
	MOTA	799 OG1 THR A 368	33.101 21.0.1
30	MOTA	800 CG2 THR A 368	36.323 23.303 33.400 31.13 6
50	MOTA	801 C THR A 368	34.764 23.337
	ATOM	802 O THR A 368	34.400 20.200 20.553 1 00 21 32 7
	MOTA	803 N GLU A 369	35.545 20.092 35.551 1.00 39 00 6
	ATOM	804 CA GLU A 369	36.065 27.455 35.662 1.00 32 79 6
35	MOTA	805 CB GLU A 369	36.960 27.707 32.100 1 00 36 29 6
	MOTA	806 CG GLU A 369	38.089 26.003 32.310 1.00 41.03
	MOTA	807 CD GLU A 369	38.906 26.747 31.120 2.00 42.05
	ATOM	808 OE1 GLU A 369	38.337 20.744 23.331
	MOTA	809 OE2 GLU A 369	40.158 20.795 51.225 1.00 25 57 6
40		810 C GLU A 369	34.955 20.471 35.022 1.00 20 56 8
	MOTA	811 O GLU A 369	34.987 29.230 34.700
	ATOM	812 N VAL A 370	33.967 20.403 32.322 1 00 05 00
	ATOM	813 CA VAL A 370	32.849 29.330 33.00 1 00 00 15 6
	MOTA	814 CB VAL A 370	31.763 29.131 31.30 07 65 6
45	MOTA	815 CG1 VAL A 370	30.609 30.093 32.730
	ATOM	816 CG2 VAL A 370	32.308 23.231 33.31
	ATOM	817 C VAL A 370	32.245 29.209 31.11
	MOTA	818 O VAL A 370	32.012 30.170 30.170 7
	ATOM	819 N ALA A 371	31.900 27.947 34.00 10 57 6
50	MOTA (820 CA ALA A 371	31.393 27.334 35.15 1 00 10 62 6
	MOTA	821 CB ALA A 371	31.441 20.033 35.49 6
	ATOM	822 C ALA A 371	32.110 20.211 3.00 32 67 8
•	MOTA	823 O ALA A 371	31.551 20.905 3.05 1.00 22 89 7
	ATOM	824 N LEU A 372	33.401 27.893 37.303
5		825 CA LEU A 372	34.217 20.447 30.000
	ATOM	826 CB LEU A 372	35.675 27.390 30.215 2.00.23 19 6
	MOTA	827 CG LEU A 372	35.943 20.324 30.3264 6
	MOTA		37.356 26.171 38.049 1.00 27.64 6

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5	ATOM	829 CD2 LEU A 372	35.675	26.204		7.00 20.90	6
J	ATOM	830 C LEU A 372	34.098	29.966	38.396	1.00 21.34	6
	ATOM	831 O LEU A 372	33.828	30.572	39.439	1.00 23.16	8
	ATOM	832 N LEU A 373	34.288	30.561	37.223	1.00 24.42	7
	ATOM	833 CA LEU A 373	34.214	32.007	37.074	1.00 23.78	6
10	ATOM	834 CB LEU A 373	34.296	32.360	35.575	1.00 22.18	6
10	MOTA	835 CG LEU A 373	34.784	33.726	35.165	1.00 31.52	6
	ATOM	836 CD1 LEU A 373	36.000	34.084	35.962	1.00 31.93	6
	ATOM	837 CD2 LEU A 373	35.103	33.720	33.693	1.00 30.24	6
		838 C LEU A 373	32.904	32.480	37.720	1.00 25.69	6
15	ATOM	839 O LEU A 373	32.895	33.410	38.532	1.00 30.13	8
15	MOTA	840 N GLN A 374	31.814	31.800	37.368	1.00 26.24	7
	MOTA	841 CA GLN A 374	30.487	32.104	37.896	1.00 21.60	6
	ATOM	842 CB GLN A 374	29.454	31.121	37.335	1.00 24.57	6
	MOTA		29.310	31.145	35.821	1.00 21.02	6
00	ATOM		28.224	30.201	35.331	1.00 22.86	6
20	ATOM		28.037	30.042	34.123	1.00 24.07	8
	MOTA		27.515	29.590	36.249	1.00 25.59	7
	MOTA		30.421	32.039	39.422	1.00 20.66	6
	ATOM	·	29.717	32.832	40.048	1.00 24.47	8
	MOTA		31.136	31.074	40.004	1.00 16.26	7
25	MOTA		31.155	30.889	41.445	1.00 17.16	6
	MOTA		31.805	29.568	41.780	1.00 19.53	6
	MOTA	851 CB ALA A 375	31.907	32.025	42.108	1.00 25.13	6
	MOTA	852 C ALA A 375	31.397	32.646	43.034	1.00 23.81	8
	MOTA	853 O ALA A 375 854 N VAL A 376	33.122	32.277	41.611	1.00 24.57	7
30	MOTA		33.959	33.354	42.118		6
	MOTA		35.101	33.658	41.164	1.00 26.48	6
	MOTA		35.926	34.812	41.697		6
	MOTA		35.959		40.952		6
	ATOM		33.107	34.599	42.312		6
35	MOTA		33.297		43.251		8
	MOTA		32.159		41.399		7
	MOTA		31.242		41.423		6
	MOTA		30.540				6
40	MOTA		31.424				6
40	ATOM		30.689				6
	MOTA		31.916				6
	MOTA		30.228				6
	ATOM		30.131				8
4.5	MOTA		29.483				7
45			28.469				6
	ATOM		28.053				6
	MOTA		27.110				6
	MOTA	872 CG LEU A 378	25.91				6
	ATOM	873 CD1 LEU A 378	26.693				6
50		874 CD2 LEU A 378	28.992				6
	MOTA	875 C LEU A 378	28.39				8
	MOTA	876 O LEU A 378					7
	MOTA	877 N MET A 379	30.11				6
	MOTA	878 CA MET A 379	30.73				6
55		879 CB MET A 379	31.69				6
	ATOM	880 CG MET A 379	30.98				16
	MOTA	881 SD MET A 379	29.74				6
	MOTA	882 CE MET A 379	28.89	0 30.03	U 47.03		-

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5		883		MET A 379		5 35.4	生 多	ジューションコージョン	-
	ATOM	884		MET A 379	32.56	7 35.45	0 47.305		•
	ATOM	885		SER A 380	30.88				
	ATOM	886			31.49				=
10	ATOM	887			30.92				-
10	ATOM	888		SER A 380	31.20				6
	ATOM	889		SER A 380	31.17				
	ATOM	890		SER A 380	30.02				6
	ATOM	891		SER A 381	. 32.21			77.03	8
	ATOM	892		SER A 381	32.06				7
15	ATOM	893		SER A 381	33.32				6
	ATOM	894		SER A 381	34.43				6
	ATOM	895		SER A 381	31.79				8
	ATOM	896	0	SER A 381	31.47				6
	ATOM	897	N	ASP A 382	31.93				8
20	ATOM	898	CA	ASP A 382	31.74				7
	ATOM	899	CB	ASP A 382	32.67				6
	ATOM	900	CG	ASP A 382	32.572				6
	ATOM	901	OD	1 ASP A 382	32.70	_			6
	ATOM	902	OD	2 ASP A 382	32.358				8
25	ATOM	903	С	ASP A 382	30.314				8
	ATOM	904	0	ASP A 382	30.048				6
	MOTA	905	N	ARG A 383	29.397				8
	ATOM	906	ÇA	ARG A 383	28.036			1.00 42.63	7
-	ATOM	907	CB	ARG A 383	27.138		48.443	1.00 43.32	6
30	MOTA	908	CG	ARG A 383	27.651		47.352	1.00 42.31	6
	ATOM	909	CD	ARG A 383	27.586		45.925	1.00 40.83	6
	ATOM	910	NE	ARG A 383	27.768		44.975	1.00 38.09 1.00 37.33	6
	ATOM	911	CZ	ARG A 383	28.037		43.693		7
25	ATOM	912	NH		28.142		43.198	1.00 38.35 1.00 33.70	6
35	ATOM	913		2 ARG A 383	28.194		42.918	1.00 35.46	7
	MOTA	914	С	ARG A 383	27.523		50.216	1.00 33.46	7
	ATOM	915	0	ARG A 383	27.744		51.260	1.00 44.98	6
	ATOM	916	N	PRO A 384	26.852		50.223	1.00 45.33	8
40	ATOM	917	CD	PRO A 384	26.625		49.027	1.00 46.85	7 6
40	ATOM	918	CA	PRO A 384	26.298	44.738	51.446	1.00 47.37	6
	ATOM	919	CB	PRO A 384	25.841	46.130	51.012	1.00 46.90	6
	ATOM	920	CG	PRO A 384	26.075	46.229	49.567	1.00 46.41	6
	ATOM	921	С	PRO A 384	25.158	43.919	52.049	1.00 48.29	6
45	ATOM	922	0	PRO A 384	24.404	43.264	51.329	1.00 48.34	8
73	ATOM	923	N	GLY A 385	25.039	43.983	53.383	1.00 49.88	7
	ATOM	924	CA	GLY A 385	23.991	43.270	54.113	1.00 50.35	6
	ATOM	925	С	GLY A 385	24.347	41.852	54.495	1.00 50.70	6
	ATOM	926	0	GLY A 385	23.614	41.204	55.244	1.00 53.48	8
50	ATOM	927	N	LEU A 386	25.466	41.371	53.955	1.00 49.04	7
50	ATOM	928	CA	LEU A 386	25.901	40.017	54.215	1.00 50.53	6
	ATOM	929	CB	LEU A 386	27.224	39.751	53.492	1.00 45.17	
	ATOM	930	CG	LEU A 386	27.152	39.592	51.993	1.00 48.26	6 6
	ATOM	931	CD1	LEU A 386	28.542	39.439	51.404	1.00 41.68	6
55	ATOM	932		LEU A 386	26.302	38.374	51.682	1.00 38.40	6
J J	ATOM	933	С	LEU A 386	26.045	39.776	55.691	1.00 52.13	6
	ATOM	934	0	LEU A 386	26.296	40.692	56.459	1.00 52.13	
	ATOM	935	N	ALA A 387	25.861	38.522	56.077	1.00 53.67	8 7
	ATOM	936	CA	ALA A 387	25.976	38.129	57.470	1.00 55.42	6
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5	ATOM	937 CB	ALA A 387	24.802	37.234		1.00 56.47	6
,	ATOM	938 C	ALA A 387	27.289	37.385		1.00 55.52	6
	ATOM	939 0	ALA A 387	28.275	37.940	58.134	1.00 53.75	8
		940 N	CYS A 388	27.273	36.120	57.253	1.00 56.03	7
	ATOM	941 CA	CYS A 388	28.412	35.236	57.370	1.00 59.57	6
• •	ATOM	•	CYS A 388	27.923		57.172	1.00 59.23	6
10	ATOM		CYS A 388	26.397	33.431	58.009	1.00 58.64	16
	MOTA	943 SG	CYS A 388	29.482	35.581	56.328	1.00 62.18	6
	ATOM	944 C	CYS A 388	29.720	34.821	55.400	1.00 67.88	8
	MOTA	945 0	VAL A 389	30.110	36.747	56.495	1.00 60.78	7
	ATOM	946 N	VAL A 389	31.173	37.212	55.590	1.00 57.70	6
15	ATOM	947 CA	VAL A 389	31.740	38.567	56.024	1.00 57.09	6
	ATOM	948 CB		32.795	39.037	55.041	1.00 59.03	6
	MOTA	949 CG		30.640	39.598	56.171	1.00 53.98	6
	MOTA	950 CG	VAL A 389	32.297	36.182	55.550	1.00 57.77	6
••	ATOM	951 C	VAL A 389	32.358	35.336	54.662	1.00 60.94	8
20	ATOM	952 O	ALA A 390	33.182	36.292	56.528	1.00 52.68	7
•	MOTA	953 N		34.347	35.431	56.684	1.00 48.41	6
	ATOM	954 CA		34.703	35.321	58.185	1.00 45.19	6
	MOTA	955 CB	ALA A 390	34.224	34.040	56.082	1.00 47.63	6
25	ATOM	956 C	ALA A 390	35.107	33.597	55.348	1.00 51.95	8
25	ATOM	957 O 958 N	ARG A 391	33.117	33.366	56.391	1.00 47.11	7
	MOTA	958 N 959 CA		32.879	32.018	55.885	1.00 51.64	6
	MOTA	959 CA 960 CB		31.520	31.498	56.383	1.00 54.22	6
	ATOM	961 CG		31.267	30.012	56.059	1.00 64.20	6
20	MOTA	961 CE		29.930	29.489	56.602	1.00 73.80	6
30	ATOM	963 NE		29.787	28.044	56.454	1.00 79.76	7
	ATOM ATOM	964 C2		30.573		57.043	1.00 84.27	6
	ATOM	965 NH		31.598		57.806	1.00 85.28	7
	ATOM	966 NI		30.340	25.840	56.849	1.00 86.84	7
35	ATOM	967 C	ARG A 391	32.922	31.986	54.358	1.00 48.18	6
33	ATOM	968 0	ARG A 391	33.494	31.080	53.756	1.00 49.57	8
	ATOM	969 N	ILE A 392	32.281		53.762	1.00 45.01	7
	ATOM	970 C		32.196		52.319	1.00 48.77	6
	ATOM	971 C	B ILE A 392	31.224	34.297	51.963	1.00 46.45	6
40	ATOM		G2 ILE A 392	31.241		50.479	1.00 42.35	6
	ATOM	973 C	G1 ILE A 392	29.791		52.402	1.00 49.69	6
	MOTA	974 C	D1 ILE A 392	28.792		52.113	1.00 51.09	6
	ATOM	975 C	ILE A 392			51.641	1.00 50.90	. 6
	MOTA	976 0				50.732		8 7
45	ATOM	977 N				52.071		6
	ATOM	978 C	A GLU A 393			51.471		6
	MOTA	979 C	B GLU A 393			52.387		6
	MOTA	980 C	G GLU A 393			51.844		6
	MOTA	981 C	D GLU A 393			52.564		8
50	MOTA		E1 GLU A 393					8
	MOTA	983 C	E2 GLU A 393					6
	MOTA	984 0						8
	MOTA	985 0						7
	ATOM	986 N						
55			CA LYS A 394					
	MOTA		CB LYS A 394					
	MOTA		CG LYS A 394					
	MOTA	990 (CD LYS A 394	39.37	2 32.374	53.705	, 1.00 40.00	J

5	ATOM	991	CE	LYS A	394	40.136	799245	54.689	1989 40.00	6
	ATOM	992	NZ	LYS A	394	41.516	33.602	54.162	1.00 40.00	7
	MOTA	993	С	LYS A	394	36.568	30.778	50.966	1.00 46.69	6
	ATOM	994	0	LYS A	394	37.215	30.427	49.988	1.00 49.13	8
	ATOM	995	N	TYR A	395	35.269	30.514	51.095	1.00 46.57	7
10	MOTA	996	CA	TYR A	395	34.553	29.823	50.022	1.00 43.33	6
	MOTA	997	CB	TYR A	395	33.059	30.123	50.076	1.00 48.44	6
	MOTA	998	CG	TYR A	395	32.275	29.236	50.994	1.00 53.83	6
	ATOM	999	CD1	TYR A	395	31.010	29.598	51.415	1.00 56.43	6
	ATOM	1000	CE1	TYR A	395	30.266	28.769	52.252	1.00 59.73	6
15	MOTA	1001	CD2	TYR A	395	32.790	28.033	51.428	1.00 56.47	6
	ATOM	1002	CE2	TYR A	395	32.054	27.198	52.265	1.00 62.60	6
	ATOM	1003	cz	TYR A	395	30.787	27.565	52.687	1.00 63.18	6
	MOTA	1004	OH	TYR A	395	30.059	26.753	53.528	1.00 64.46	8
	MOTA	1005	С	TYR A	395	35.120	30.356	48.716	1.00 37.30	6
20	MOTA	1006	0	TYR A	395	35.643	29.601	47.908	1.00 34.10	8
	MOTA	1007	N	GLN A	396	35.029	31.670	48.522	1.00 31.92	7
	ATOM	1008	CA	GLN A		35.563	32.273	47.305	1.00 34.81	6
	MOTA	1009	CB	GLN A	396	35.403	33.801	47.329	1.00 32.64	6
	ATOM	1010	CG	GLN A	396	36.088	34.485	46.162	1.00 29.57	6
25	MOTA	1011	CD	GLN A	396	35.616	35.891	45.927	1.00 29.46	6
	ATOM	1012	OE1	GLN A	396	35.599	36.726	46.862	i.00 34.65	8
	MOTA	1013	NE2	GLN A	396	35.245	36.173	44.689	1.00 27.21	7
	MOTA	1014	C	GLN A	396	37.035	31.909	47.167	1.00 37.13	6
	ATOM	1015	0	GLN A	396	37.511	31.590	46.080	1.00 37.36	8
30	MOTA	1016	N	ASP A	397	37.751	31.970	48.285	1.00 38.61	7
	MOTA	1017	CA	ASP A	397	39.164	31.642	48.298	1.00 40.37	6
	MOTA	1018	CB	ASP A	397	39.757	31.869	49.704	1.00 40.51	6
	MOTA	1019	CG	ASP A	397	39.813	33.319	50.095	1.00 43.77	6
	MOTA	1020	OD1	ASP A	397	40.397	34.123	49.334	1.00 46.50	8
35	MOTA	1021	OD2	ASP A	397	39.299	33.702	51.184	1.00 51.34	8
	MOTA	1022	С	ASP A	397	39.302	30.176	47.898	1.00 38.62	6
	ATOM	1023	0	ASP A	397	40.230	29.809	47.199	1.00 39.20	8
	MOTA	1024	N	SER A	398	38.350	29.359	48.344	1.00 37.84	7
	MOTA	1025	CA	SER A	398	38.348	27.929	48.063	1.00 37.80	6
40	MOTA	1026	CB	SER A		37.240	27.240	48.878	1.00 34.28	6
	ATOM	1027	OG	SER A		37.297	25.826	48.755	1.00 46.60	8
	MOTA	1028	С	SER A		38.164	27.639	46.581	1.00 38.41	6
	MOTA	1029	0	SER A		38.677	26.642	46.075	1.00 39.98	8
	ATOM	1030	N	PHE A		37.419	28.507	45.893	1.00 34.82	7
45	ATOM	1031	CA	PHE A		37.181	28.325	44.462	1.00 35.96	6
	MOTA	1032	CB	PHE A		35.873	28.983	44.015	1.00 35.75	6
	MOTA	1033	CG	PHE A		34.632	28.216	44.403	1.00 39.30	6
	ATOM	1034	CD1			34.107	28.294	45.677	1.00 39.86	6
	ATOM	1035		PHE A		34.018	27.393	43.488	1.00 36.81	6
50	ATOM	1036	CEl			32.961	27.557	46.013	1.00 41.25	6
	ATOM	1037	CE2			32.880	26.661	43.825	1.00 43.61	6
	MOTA	1038	CZ	PHE A		32.354	26.740	45.087	1.00 40.34	6
	ATOM	1039	С	PHE A		38.328	28.890	43.630	1.00 33.48	6
_ =	ATOM	1040	0	PHE A		38.867	28.200	42.756	1.00 26.86	8
55	ATOM	1041	N	LEU A		38.680	30.156	43.877	1.00 31.47	7
	MOTA	1042	CA	LEU A		39.754	30.796	43.132	1.00 37.41	6
	MOTA	1043	СВ	LEU A		40.179	32.100	43.814	1.00 34.24	6
	MOTA	1044	CG	LEU A	400	39.239	33.265	43.628	1.00 35.10	6

	WO 99/	060014								PCT/US99/06899	
5	ATOM	1045	CD1	LEU	А	400	39.803	34.531	44.256	1.00 26.60	6
	ATOM	1046		LEU			39.065	33.479	42.137	1.00 29.44	6
	ATOM	1047	С	LEU			40.941	29.872	42.947	1.00 38.84	6
	ATOM	1048	0	LEU			41.367	29.632	41.821	1.00 40.38	8
	ATOM	1049	N	LEU			41.464	29.350	44.055	1.00 42.79	7
10	ATOM	1050	CA	LEU			42.605	28.449	43.988	1.00 42.79	
- 0	ATOM	1051	CB			401	42.900	27.821	45.355	1.00 43.48	6
	MOTA	1052	CG	LEU			44.105	26.899	45.354		6
	ATOM	1052		LEU			45.374			1.00 51.39	6
	ATOM	1053	CD2					27.749	45.143	1.00 50.11	6
15	ATOM	1055					44.205	26.122	46.662	1.00 49.30	6
13		1055	С	LEU			42.324	27.340	42.981	1.00 41.62	6
	ATOM		0			401	43.052	27.180	42.004	1.00 45.14	8
	ATOM	1057	N	ALA			41.269	26.574	43.245	1.00 37.92	7
	ATOM	1058	CA			402	40.873	25.469	42.386	1.00 29.90	6
20	ATOM	1059	CB	ALA			39.522	24.928	42.834	1.00 30.70	6
20	ATOM	1060	С	ALA			40.798	25.909	40.929	1.00 28.88	6
	ATOM	1061	0	ALA			41.277	25.203	40.034	1.00 32.14	8
	MOTA	1062	N	PHE			40.200	27.086	40.707	1.00 31.07	7
	MOTA	1063	CA			403	40.052	27.642	39.363	1.00 29.90	6
0.5	MOTA	1064	CB			403	39.379	29.019	39.438	1.00 27.03	6
25	MOTA	1065	CG			403	38.943	29.574	38.100	1.00 26.97	6
	MOTA	1066		PHE			38.228	30.758	38.033	1.00 25.55	6
	MOTA	1067		PHE			39.224	28.905	36.925	1.00 19.75	6
	MOTA	1068		PHE			37.784	31.266	36.808	1.00 27.90	6
	MOTA	1069		PHE			38.780	29.416	35.694	1.00 22.56	6
30	MOTA	1070	CZ			403	38.063	30.596	35.640	1.00 22.24	6
	MOTA	1071	С			403	41.429	27.756	38.719	1.00 28.82	6
	MOTA	1072	0			403	41.666	27.210	37.646	1.00 26.00	8
	MOTA	1073	N	GLU			42.329	28.463	39.402	1.00 30.25	7
	MOTA	1074	CA	GLU			43.695	28.665	38.922	1.00 34.03	6
35	MOTA	1075	CB	GLU			44.513	29.416	39.983	1.00 39.45	6
	MOTA	1076	CG	GLU			45.867	29.935	39.489	1.00 47.68	6
	MOTA	1077	CD	GLU			46.734	30.507	40.571	1.00 54.02	6
	MOTA	1078	OE1				46.236	31.298	41.408	1.00 57.27	8
40	ATOM	1079	OE2	GLU			47.956	30.202	40.606	1.00 63.85	8
40	MOTA	1080	С	GLU			44.352	27.322	38.634	1.00 36.01	6
	ATOM	1081	0	GLU			44.936	27.112	37.574	1.00 38.64	8
	MOTA	1082	N	HIS			44.259	26.420	39.610	1.00 29.56	7
	MOTA	1083	CA	HIS			44.840	25.093	39.468	1.00 31.69	6
4.5	MOTA	1084	CB	HIS			44.540	24.228	40.694	1.00 33.75	6
45	MOTA	1085	CG				45.292	24.657	41.908	1.00 34.75	6
	ATOM	1086		HIS			46.198	25.640	42.130	1.00 34.58	6
	ATOM	1087		HIS			45.161	23.984	43.130	1.00 32.43	7
	MOTA	1088		HIS			45.975	24.568	44.018	1.00 36.15	6
~~	MOTA	1089		HIS			46.601	25.561	43.430	1.00 39.84	7
50	MOTA	1090	С	HIS			44.274	24.445	38.225	1.00 34.21	6
	ATOM	1091	0	HIS			45.029	23.949	37.386	1.00 37.06	8
	ATOM	1092	N	TYR			42.947	24.453	38.100	1.00 30.83	7
	MOTA	1093	CA	TYR			42.313	23.859	36.930	1.00 28.85	6
	ATOM	1094	CB	TYR			40.805	24.080	36.934	1.00 31.48	6
55	ATOM	1095	CG	TYR			40.139	23.494	35.709	1.00 23.49	6
	MOTA	1096		TYR			40.073	22.123	35.532	1.00 19.42	6
	MOTA	1097		TYR			39.517	21.577	34.382	1.00 23.80	6
	MOTA	1098	CD2	TYR	Α	406	39.646	24.313	34.704	1.00 21.81	6

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		1099			A 406		23 - 6	AUS : £5.	JE. 64	6
	ATOM	1100			A 406		22.395	33.380	1.00 21.56	
	ATOM	1101			A 406		21.850			
	MOTA	1102			A 406		24.504			6
	ATOM	1103		TYR	A 406	42.958				8
10	ATOM	1104	N	ILE	A 407					
	MOTA	1105	CA	ILE	A 407					
	ATOM	1106	CB	ILE	A 407	43.986				6
	ATOM	1107	CG2		A 407	44.967				6
	ATOM	1108			A 407	42.615				6
15	ATOM	1109			A 407	41.896				6
	ATOM	1110			A 407	45.143				6
	ATOM	1111	o		A 407					6
	ATOM	1112			A 408	45.383				8
	ATOM	1113	CA		A 408	46.003	_			7
20	ATOM	1114				47.307				6
20	ATOM	1115	CB		A 408	48.107			1.00 32.27	6
	ATOM		CG		A 408	48.346		36.936		6
		1116		ASN .		48.827	• •	36.320	1.00 31.99	8
	ATOM	1117		ASN .		48.038	26.403	38.231		7
25	ATOM	1118	С		A 408	47.205	23.892			6
25	ATOM	1119	0		A 408	47.900	23.734			8
	ATOM	1120	N		A 409	46.334	22.981	34.568		7
	ATOM	1121	CA	TYR :	A 409	46.159	21.710	33.866		6
	ATOM	1122	CB	TYR I	A 409	45.051	20.859	34.507	1.00 33.91	
	ATOM	1123	CG	TYR Z	A 409	44.624	19.687	33.619	1.00 34.41	6
30	MOTA	1124	CD1	TYR Z	A 409	45.563	18.765	33.155	1.00 38.73	6
	MOTA	1125	CE1	TYR A	A 409	45.186	17.709	32.321		6
	MOTA	1126	CD2			43.292	19.515	33.232	1.00 47.16	6
	MOTA	1127	CE2			42.913	18.455	32.397	1.00 46.20	6
	ATOM	1128	cz		A 409	43.863	17.551		1.00 50.74	6
35	ATOM	1129			A 409	43.498		31.946	1.00 50.88	6
	ATOM	1130	С	TYR A		45.760	16.514	31.130	1.00 53.14	8
	ATOM	1131	0	TYR A		46.202	21.966	32.424	1.00 38.16	6
	MOTA	1132	N	ARG A			21.281	31.502	1.00 41.83	8
	ATOM	1133	CA	ARG A		44.872	22.943	32.272	1.00 42.25	7
40	ATOM	1134	CB	ARG A		44.345	23.332	30.984	1.00 42.83	6
	ATOM	1135	CG	ARG A		43.311	24.427	31.195	1.00 36.83	6
	ATOM	1136	CD	ARG A		41.994	23.979	31.795	1.00 34.32	6
	ATOM	1137	NE			41.073	23.504	30.675	1.00 36.62	6
	ATOM	1138	CZ	ARG A		40.888	24.550	29.685	1.00 38.64	7
45	ATOM	1139		ARG A		40.177	24.397	28.576	1.00 35.73	6
	ATOM	1140		ARG A		39.572	23.230	28.348	1.00 33.17	7
	ATOM			ARG A		40.077	25.407	27.708	1.00 32.70	7
	ATOM	1141	C	ARG A		45.442	23.850	30.083	1.00 46.67	6
		1142	0	ARG A		45.467	23.591	28.882	1.00 41.78	8
50	ATOM	1143	N	LYS A		46.360	24.577	30.710	1.00 52.99	7
50	ATOM	1144	CA	LYS A		47.467	25.194	30.017	1.00 58.32	6
	ATOM	1145	CB	LYS A		48.645	24.216	29.876	1.00 64.99	6
	MOTA	1146	CG	LYS A	411	48.349	22.835	29.367	1.00 70.48	
	MOTA	1147	CD	LYS A		49.608	21.974	29.494	1.00 70.48	6
5.5	MOTA	1148	CE	LYS A	411	49.461	20.621	28.795		6
55	ATOM	1149	NZ	LYS A		50.740	19.828	28.857	1.00 84.30	6
	MOTA	1150		LYS A		47.032	25.756	28.686	1.00 86.48	7
	MOTA	1151		LYS A		47.160	25.758		1.00 56.66	6
	ATOM	1152		HIS A		46.458	26.943	27.633	1.00 55.47	8
					-	40.400	20.343	28.823	1.00 54.67	7

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WO 99/060014	27.705 1.00 48.67 6
5 NEOM 1153 CA HIS A 412	45.984 27.722 27.705 1.00 13.10 6
3 AIOM 110	45.124 28.884 28.201 1.00 43.26
ATOM TTO	43 812 28.480 28.755 1.00 31.00
ATOM 1155 CG HIS A 412	42 429 28.064 29.967 1.00 33.11
1156 CD2 HIS A 412	42 651 28.440 27.966 1.00 38.19
NUON 1157 ND1 HIS A 412	28.723 1.00 34.75
10 2 POM 1158 CE1 HIS A 412	41.040 27.780 29.942 1.00 35.52
10 A1011	42.034 27.101 1.00 46.35 6
A10th	47.231 28.303 27 775 1 00 42 73 8
ATOM 1100 D UTS A 412	48.269 26.432 25.030 1.00 48.92 7
A10M N UTS A 413	47.116 20.030 25 146 1 00 53 15 6
ATOM CD UTS A 413	48.234 29.290 25.146 1.00 55 27 6
15 ATOM 113	48.404 28.666 23.755 1.00 50 77 6
AIOM 110	49 326 29.446 22.886 1.00 30.77
ATOM 1165 CG HIS A 413	49 213 30.660 22.304 1.00 01.00
NROM 1166 CD2 HIS A 413	50 617 28.997 22.564 1.00 00.01
7 MON 1167 ND1 HIS A 413	51 214 29.924 21.828 1.00 63.01
20 AMOM 1168 CE1 HIS A 413	20 20 21 658 1.00 62.93
20 NEOM 1169 NE2 HIS A 413	30.300 20.768 24.998 1.00 53.19 6
2001 1170 C HIS A 413	27.552 21 301 23.934 1.00 54.93 8
7 MOM 1171 O HIS A 413	7.000 21 413 26.139 1.00 53.77
NTOM 1172 N VAL A 414	47.904 32.011 26 146 1.00 51.06 6
ATOM 1172 CA WAT A 414	47.735 32.011 26.417 1.00 51.49 6
25 A10M 1170	46.291 33.103 26.602 1 00 45 22 6
ATOM TITE ACT STAT A A14	46.186 34.713 25.262 1 00 52.67 6
A10H	45.419 32.732 20.00 1 00 54.28 6
A1011 A 414	48.623 33.203 23.400 1.00 55.49 8
A10M 1170 O 7/AT. A 414	48.427 33.023 200 56.28 7
30 A10M 1270 mup A 415	49.706 33.003 27.57 1.00 57.83 6
AIOM 11.	50.721 34.484 27.557 1.00 57.60
AIOM 1100	51.268 35.675 26.738 1.00 35.65
Alon 1101	51.605 36.754 27.636 1.00 60.65
AIOM IIIO	50 197 36.158 25.745 1.00 JJ.12
35 ATOM 1183 CG2 THR A 415.	50 146 35.049 28.879 1.00 30.70
ATOM 1184 C THR A 415	49 933 35.146 29.051 1.00 33.1
ATOM 1185 O THR A 415	51 068 35.330 29.795 1.00 57.44
NEON 1186 N HIS A 416	50 808 36.011 31.047 1.00 37.34
ATOM 1187 CA HIS A 416	51 346 37.422 30.708 1.00 61.33
10 RECM 1188 CB HIS A 416	31.821 1.00 69.76
70M 1189 CG HIS A 410	32 327 32 390 1.00 /1.42
1190 CD2 HIS A 410	20 263 32 416 1.00 /2.49
NTOM 1191 ND1 HIS A 416	31.133 30.884 33.290 1.00 75.50 6
NTOM 1192 CE1 HIS A 416	31.914 33.091 1.00 73.91
45 DTOM 1193 NE2 HIS A 416	35.053 35.892 31.297 1.00 53.79
ATOM 1194 C HIS A 416	49.201 30.779 30.902 1.00 52.81 8
ATOM TITE A 416	48.499 36.779 30.00 48.05 7
AIOM TIPE A 417	48.806 34.775 22.061 1.00.47.99 6
AIOM AIO DUE A A17	47.355 34.426 31.00 46.11 6
ATOM THE A 417	47.165 32.934 31.300 1.00 44.27 6
30 AIOH 117	45.835 32.336 32.046 1 00 41.79 6
AIOM TENE ADI DUE A 417	45.680 32.720 30.040 1.00 40.23 6
GD3 DUE A 417	44.758 32.135 32.104 1.00 44.30 6
ATOM OF DUE A 417	44.498 32.397 29.422 1.00 44.30
A1011 7 /17	43.540 31.802 31.529 1.00 30.00
55 ATOM 1203 CE2 PHE A 417	43.427 31.928 30.144 1.00 40.69 6
ATOM 1204 CZ PHE A 417	46.427 34.836 33.196 1.00 46.69
ATOM 1205 C PHE A 417	26 004 33 331 1.00 43.33
ATOM 1206 O PHE A 417	

5	ATCM	1207	N	TRP	A	418	45.906	33.801	33.909	1.00	45.14	7
	ATOM	1208	CA	TRP	A	418	44.982	33.867	35.065		44.89	6
	ATOM	1209	CB	TRP	A	418	45.545	33.099	36.255		42.24	6
	ATOM	1210	CG	TRP	Α	418	44.959	33.452	37.598		47.11	6
	ATOM	1211	CD2	TRP	Α	418	43.724	32.924	38.149		46.98	6
10	ATOM	1212	CE2	TRP	A	418	43.534	33.565	39.413		48.94	6
	MOTA	1213	CE3	TRP	Α	418	42.777	31.986	37.688		45.23	6
	ATOM	1214	CD1			418	45.434	34.350	38.512		46.24	
	MOTA	1215	NE1			418	44.588	34.407	39.608		50.63	6
	MOTA	1216	CZ2			418	42.441	33.270	40.238		45.46	7
15	MOTA	1217	CZ3			418	41.686	31.706	38.500		44.50	6
	ATOM	1218	CH2			418	41.511	32.335	39.753		47.55	6
	MOTA	1219	С			418	44.908	35.324	35.398		47.33	6
	MOTA	1220	0			418	43.797	35.839	35.702			6
	MOTA	1221	N			419	46.084	35.976	35.461		43.17 43.55	8
20	ATOM	1222	CD			419	47.467	35.482	35.400			7
	ATOM	1223	CA			419	46.009	37.396	35.758	1.00		6
	ATOM	1224	СВ			419	47.436	37.884			41.48	6
	ATOM	1225	CG			419	48.261	36.696	35.535	1.00		6
	ATOM	1226	C			419	44.960	38.090	35.223	1.00		6
25	ATOM	1227	0			419	44.208	38.978	34.817	1.00		6
	MOTA	1228	N			420	44.915	37.701	35.237		37.08	8
	MOTA	1229	CA			420	43.977	38.287	33.540	1.00		7
	ATOM	1230	CB			420	44.314		32.575		40.82	6
	ATOM	1231	CG			420	45.684	37.805	31.155		40.78	6
30	ATOM	1232	CD			420	45.904	38.244	30.641		48.62	6
	MOTA	1233	CE			420	47.248	37.781	29.206		55.12	6
	MOTA	1234	NZ			420	47.448	38.261 37.884	28.673		53.26	6
	ATOM	1235	C	LYS			42.580	37.832	27.222		52.69	7
	MOTA	1236	Ö	LYS			41.656	38.626	32.948 32.982		40.29	6
35	ATOM	1237	N	LEU			42.461	36.537			39.66	8
	MOTA	1238	CA	LEU			41.186	35.931	33.245		38.33	7
	ATOM	1239	CB	LEU			41.397	34.433	33.613 33.915	1.00		6
	ATOM	1240	CG	LEU			40.204	33.518	33.828		43.66	6
	ATOM	1241	CD1	LEU			39.643	33.624	32.426		46.50	6
40	ATOM	1242	CD2	LEU			40.595	32.094	34.131	1.00	45.15	6
	MOTA	1243	C	LEU			40.575	36.664	34.131	1.00	51.31 39.59	6
	ATOM	1244	Ō	LEU			39.371	36.910	34.837		40.66	6
	ATOM	1245	N	LEU			41.412	37.017	35.782		39.57	8
	MOTA	1246	CA	LEU			40.946	37.726	36.961		39.57	7
45	ATOM	1247	СВ	LEU			42.085	37.720	37.971		41.79	6
	ATOM	1248	CG	LEU			42.424	36.671	38.798		42.74	6
	ATOM	1249		LEU			43.490	37.010	39.820			6
	MOTA	1250		LEU			41.168	36.216	39.523		42.89	6
	MOTA	1251	c	LEU			40.381	39.073			39.27	6
50	ATOM	1252	Ō	LEU			39.428	39.525	36.589		40.47	6
	ATOM	1253	N	MET			40.969		37.210		47.83	8
	ATOM	1254	CA	MET			40.511	39.698	35.569		34.27	7
	ATOM	1255	СВ	MET			41.427	41.001	35.117		35.25	6
	ATOM	1256		MET				41.553	34.028		32.56	6
55	ATOM	1257	SD	MET			42.856	41.732	34.456		40.70	6
	ATOM	1257		MET			43.707	43.101	33.619		47.65	16
	ATOM	1259		MET			43.348	42.776	31.848		47.16	6
	ATOM	1260		MET			39.100	40.899	34.574		35.13	6
	011	1200	J	rate 1	M	423	38.315	41.829	34.696	1.00	29.85	8

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5	ATOM	1261	N	LYS A	. 42	4	38.791	39.752	33.975	1.00	31.56	7
	ATOM	1262	CA	LYS A	42	4	37.470	39.529	33.423		32.29	6
	ATOM	1263	CB	LYS A	. 42	4	37.446	38.205	32.658	1.00	30.56	6
	ATOM	1264	CG	LYS A	42	4	38.394	38.192	31.455	1.00	30.07	6
	ATOM	1265	CD	LYS P	42	4	38.050	39.326	30.488	1.00	33.22	6
10	ATOM	1266	CE	LYS A	42	4	39.032	39.433	29.322	1.00	28.75	6
	ATOM	1267	NZ	LYS F	42	4	40.394	39.942	29.707	1.00	31.01	7
	ATOM	1268	С	LYS A	42	24	36.418	39.558	34.524	1.00	29.26	6
	ATOM	1269	0	LYS F			35.307	39.998	34.289	1.00	30.22	8
	ATOM	1270	N	VAL A			36.796	39.098	35.719	1.00	23.53	7
15	ATOM	1271	CA	VAL A			35.897	39.107	36.866	1.00	28.91	6
	ATOM	1272	СВ	VAL A			36.541	38.460	38.094	1.00	29.44	6
	ATOM	1273	CG1	VAL A			35.673	38.642	39.320	1.00	28.81	6
	ATOM	1274	CG2	VAL A			36.764	36.985	37.849	1.00	31.22	6
	ATOM	1275	C	VAL A			35.512	40.548	37.161	1.00	32.03	6
20	ATOM	1276	Ó	VAL A			34.350	40.839	37.429	1.00	31.95	8
20	ATOM	1277	N	THR A			36.496	41.444	37.124	1.00	33.61	7
	ATOM	1278	CA	THR Z			36.248	42.866	37.356	1.00	30.76	6
	MOTA	1279	CB	THR A			37.559	43.670	37.360	1.00	32.34	6
	ATOM	1280	OG1	THR Z			38.209	43.565	38.630		33.07	8
25	ATOM	1281	CG2	THR A			37.302	45.131	37.015		25.40	6
45	MOTA	1282	C	THR 2			35.363	43.324	36.211	1.00	32.53	6
	ATOM	1283	0	THR 2			34.357	44.006	36.405	1.00	35.19	8
	ATOM	1284	N	ASP :			35.763	42.929	35.006	1.00	28.83	7
	MOTA	1285	CA	ASP 2			35.011	43.272	33.810	1.00	35.12	6
30	ATOM	1286	CB	ASP			35.556	42.524	32.578	1.00	39.14	6
30	ATOM	1287	CG	ASP .			36.837	43.103	32.057		45.80	6
	ATOM	1288	OD1	ASP .			36.982	44.346	32.024		41.97	8
	MOTA	1289		ASP .			37.735	42.333	31.616		50.06	8
	ATOM	1290	C	ASP .			33.537	42.925	34.028		33.94	6
35	MOTA	1291	0	ASP .			32.659	43.712	33.702		38.02	8
33	MOTA	1292	N	LEU			33.283	41.745	34.584	1.00		7
	ATOM	1293	CA	LEU			31.925	41.293	34.850	1.00		6
	ATOM	1294	СВ	LEU			31.924	39.786	35.133		22.49	6
	ATOM	1295	CG	LEU			32.104	38.873	33.939		25.54	6
40	ATOM	1296	CD1	LEU			32.202	37.421	34.353		20.60	6
	ATOM	1297		LEU			30.920	39.083	33.029	1.00	17.24	6
	MOTA	1298	C	LEU			31.276	42.057	35.991		28.94	6
	ATOM	1299	Ō	LEU			30.082	42.306	35.939		31.26	8
	ATOM	1300	N	ARG			32.059	42.423	37.011		27.64	7
45	ATOM	1301	CA	ARG			31.527	43.162	38.147	1.00	28.13	6
	MOTA	1302	CB	ARG			32.564	43.298	39.264	1.00	29.59	6
	ATOM	1303	CG	ARG			32.818	42.040	40.080		34.85	6
	MOTA	1304	CD	ARG			33.588	42.360	41.367	1.00	47.18	6
	ATOM	1305	NE	ARG			34.093	41.175	42.049		57.93	7
50	ATOM	1306	CZ	ARG			33.327	40.210	42.547		63.62	6
	ATOM	1307		ARG			31.998	40.270	42.396	1.00	60.71	7
	ATOM	1308		ARG			33.900	39.165	43.150		62.38	7
	MOTA	1309	C	ARG			31.099	44.536	37.707		29.81	6
	ATOM	1310	ō	ARG			30.044	45.009	38.101		30.81	8
55	ATOM	1311	N	MET			31.941	45.176	36.901		29.64	7
50	ATOM	1312	CA	MET			31.644	46.502	36.383		34.72	6
	ATOM	1313	CB	MET			32.745	46.955	35.434		34.97	6
	ATOM	1314	CG	MET			33.937	47.597	36.080		45.34	6
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							49.120	56.000	3 00 E0 EE	1.0
5	ATOM	1315		MET A		33.520				16
	ATOM	1316		MET A		32.942	50.174	35.585	1.00 55.56	6
	ATOM	1317		MET A		30.315	46.455	35.634	1.00 34.01	6
	MOTA	1318	0	MET A	430	29.455	47.295	35.854	1.00 37.29	8
	ATOM	1319	N	ILE A	431	30.180	45.468	34.740	1.00 29.99	7
10	ATOM	1320		ILE A		28.954	45.269	33.969	1.00 28.82	6
	ATOM	1321	СВ	ILE A		28.962	43.936	33.211	1.00 27.39	6
	ATOM	1322		ILE A		27.622	43.671	32.572	1.00 23.87	6
	ATOM	1323	CG1	ILE A		30.044	43.920	32.138	1.00 25.56	6
		1324		ILE A		29.989	42.703	31.244	1.00 17.29	6
1.5	ATOM			ILE A		27.769	45.269	34.907	1.00 29.49	6
15	MOTA	1325	С	ILE A		26.810	45.993	34.712	1.00 24:19	8
	ATOM	1326	0			27.839	44.435	35.936	1.00 25.25	7
	MOTA	1327	N	GLY A			44.343	36.890	1.00 30.38	6
	ATOM	1328	CA	GLY A		26.748			1.00 30.30	6
	ATOM	1329	С	GLY A		26.494	45.671	37.554		8
20	MOTA	1330	0	GLY A		25.411	46.206	37.469	1.00 36.38	
	MOTA	1331	N	ALA A		27.514	46.189	38.221	1.00 26.77	7
	ATOM	1332	CA	ALA A	433	27.428	47.459	38.910	1.00 26.48	6
	MOTA	1333	CB	ALA A	433	28.836	47.970	39.203	1.00 19.90	6
	MOTA	1334	С	ALA A	433	26.663	48.502	38.114	1.00 30.73	6
25	ATOM	1335	0	ALA A	433	25.773	49.164	38.635	1.00 31.60	8
	ATOM	1336	N	CYS A	434	27.027	48.654	36.854	1.00 33.22	7
	ATOM	1337	CA	CYS A		26.371	49.616	35.996	1.00 34.34	6
	ATOM	1338	CB	CYS A		27.047	49.612	34.711	1.00 35.20	6
	ATOM	1339	SG	CYS A		27.789	50.811	34.285	1.00 54.48	16
30	ATOM	1340	C.	CYS A		24.974	49.198	35.612	1.00 34.09	6
30	MOTA	1341	0	CYS A		24.107	50.040	35.415	1.00 34.89	8
	ATOM	1342	N	HIS A		24.756	47.898	35.447	1.00 34.30	7
		1342	CA	HIS A		23.453	47.423	35.042	1.00 35.44	6
	MOTA	1343	CB	HIS F		23.404	45.904	35.104	1.00 31.76	6
25	ATOM		CG	HIS F		22.099	45.351	34.675	1.00 32.03	6
35	ATOM	1345				21.697	44.790	33.519	1.00 28.61	6
	MOTA	1346		HIS A		20.941	45.482	35.452	1.00 28.48	7
	ATOM	1347		HIS A		19.912	45.025	34.759	1.00 33.27	6
	ATOM	1348		HIS A			44.597	33.583	1.00 33.27	7
	MOTA	1349	NE2			20.345		35.972	1.00 31.37	6
40	MOTA	1350	С	HIS A		22.400	47.974	35.565	1.00 32.74	8
	ATOM	1351	0	HIS A		21.304	48.284		1.00 32.87	7
	ATOM	1352	N	ALA A		22.777	48.046	37.241		
	MOTA	1353	CA		A 436	21.910	48.563	38.266	1.00 29.91	6
	MOTA	1354	CB		436	22.661	48.595	39.580	1.00 21.23	6
45	MOTA	1355	С		A 436	21.475	49.969	37.884	1.00 33.86	6
	MOTA	1356	0		A 436	20.296	50.298	37.910	1.00 36.10	8.
	ATOM	1357	N	SER A	A 437	22.453	50.795	37.532	1.00 35.19	7
	MOTA	1358	CA	SER 2	A 437	22.172	52.167	37.140	1.00 33.03	6
	ATOM	1359	СВ	SER 3	A 437	23.441	52.815	36.603	1.00 35.31	6
50	ATOM	1360	OG	SER :	A 437	23.203	54.151	36.193	1.00 44.99	8
	ATOM	1361	C		A 437	21.110	52.158	36.055	1.00 38.39	6
	ATOM	1362			A 437	20.049	52.745	36.204	1.00 37.54	8
	MOTA	1363			A 438	21.432	51.483	34.956	1.00 37.32	7
	ATOM	1364			A 438	20.534	51.379	33.821	1.00 39.30	6
55		1365			A 438	21.114	50.402	32.786		6
55	ATOM				A 438	22.343		32.700		6
	ATOM	1366				21.955		31.251	1.00 45.23	6
	ATOM	1367			A 438			30.237	1.00 45.66	7
	MOTA	1368	NE	AKG	A 438	20.964	31.039	30.237	1.00 10.00	

5	ATOM	1369	CZ	ARG A	438	20.063	52.71	JUS9.	نافد نه د	゙ ! ゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚゚	6
	ATOM	1370	NH1	ARG A	438	20.046	53.958	30.318	1.00	50.91	7
	ATOM	1371	NH2	ARG A	438	19.198	52.354	28.865	1.00	45.86	7
	ATOM	1372	С	ARG A	438	19.147	50.922	34.240	1.88	42.37	6
	ATOM	1373	0	ARG A	438	18.147	51.297	33.625	1.00		8
10	MOTA	1374	N	PHE A	439	19.080	50.120	35.298	1.00		7
	ATOM	1375	CA	PHE A	439	17.803	49.624	35.763			6
	ATOM	1376	CB	PHE A		17.975	48.794	37.013		42.18	6
	ATOM	1377	CG	PHE A		16.739	48.053	37.413			6
	MOTA	1378	CD1	PHE A		16.198	47.111	36.562	1.00	47.09	6
15	ATOM	1379	CD2	PHE A		16.105	48.320	38.613	1.00	39.76	6
	ATOM	1380	CE1	PHE A		15.047	46.427	36.905	1.00	49.17	6
	MOTA	1381	CE2	PHE A		14.940	47.630	38.963	1.00	45.10	6
	MOTA	1382	CZ	PHE A		14.411	46.683	38.098	1.00	46.36	6
	ATOM	1383	С	PHE A		16.921	50.803	36.075	1.00	44.79	6
20	ATOM	1384	0	PHE A		15.830	50.903	35.554	1.00	40.26	
	ATOM	1385	N	LEU A		17.410	51.681	36.951	1.00	42.77	8
	ATOM	1386	CA	LEU A		16.660	52.871	37.344	1.00	42.77	7
	ATOM	1387	CB	LEU A		17.546	53.824	38.150	1.00	37.19	6
	ATOM	1388	CG	LEU Z		17.943		39.500	1.00	36.97	6
25	ATOM	1389	CD1	LEU F		18.620	54.389	40.316	1.00	33.65	6
	ATOM	1390	CD2	LEU A		16.679	52.837	40.216	1.00	35.42	6
	ATOM	1391	C	LEU A		16.025	53.596	36.168	1.00	45.47	6
	ATOM	1392	ō	LEU A		14.809	53.750	36.126	1.00		6
	ATOM	1393	N	HIS F		16.836	54.060	35.223	1.00	52.48 49.15	8 7
30	ATOM	1394	CA	HIS F		16.277	54.725	34.063	1.00	54.76	
	ATOM	1395	СВ	HIS F		17.329	54.955	33.031	1.00	56.68	6
	ATOM	1396	CG	HIS F		18.134	56.161	33.282	1.00	62.73	6 6
	ATOM	1397	CD2	HIS F		18.468	57.216	32.499	1.00	65.73	6
	ATOM	1398		HIS F		18.701	56.431	34.538	1.00	66.01	7
35	ATOM	1399		HIS F		19.332	57.594	34.473	1.00	65.55	6
	MOTA	1400	NE2	HIS F		19.205	58.085	33.255	1.00	60.09	7
	ATOM	1401	С	HIS F		15.244	53.822	33.481	1.00	55.93	6
	ATOM	1402	0	HIS F		14.149	54.263	33.170	1.00	57.33	8
	MOTA	1403	N	MET F		15.605	52.549	33.313	1.00	57.81	7
40	ATOM	1404	CA	MET P		14.661	51.583	32.778	1.00	59.11	6
	ATOM	1405	CB	MET P		15.191	50.154	32.922	1.00	55.93	6
	ATOM	1406	CG	MET A		16.336	49.813	32.022		58.52	6
	MOTA	1407	SD	MET A		16.681	48.008	31.851		60.99	16
	MOTA	1408	CE	MET P		17.085	47.602	33.581		52.61	6
45	MOTA	1409	С	MET A	442	13.339	51.727	33.534		60.31	6
	MOTA	1410	0	MET A	442	12.266	51.560	32.968		58.18	8
	MOTA	1411	N	LYS A	443	13.425	52.054	34.818		61.45	7
	MOTA	1412	CA	LYS A	443	12.236	52.202	35.626		64.90	6
	ATOM	1413	СВ	LYS A	443	12.608	52.141	37.090		64.40	6
50	ATOM	1414	CG	LYS A	443	11.461	51.748	37.959		69.12	6
	MOTA	1415	CD	LYS A	443	12.068	51.551	39.257		71.14	6
	ATOM	1416	CE	LYS A	443	11.368	51.897	40.091		73.43	6
	MOTA	1417	NZ	LYS A	443	11.883	51.712	41.415		67.97	7
	MOTA	1418	С	LYS A		11.513	53.514	35.348		67.29	6
55	MOTA	1419	0	LYS A		10.390	53.700	35.780		67.90	8
	MOTA	1420	N	VAL A		12.171	54.429	34.629		66.57	7
	ATOM	1421	CA	VAL A		11.575	55.719	34.297		64.76	6
	ATOM	1422	СВ	VAL A		12.569	56.869	34.560		62.76	6
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5	MOTA	1423		VAL			11.952	58.195 ^a			64 1 833	_
	MOTA	1424	CG2	VAL			12.999	56.891	36.035	1.00		6
	MOTA	1425	С	VAL			11.043	55.730	32.861		68.61	6
	MOTA	1426	0	VAL			9.937	56.210	32.612		70.60	8
	MOTA	1427	N	GLU			11.814	55.173	31.935		70.71	7
10	MOTA	1428	CA	GLU			11.457	55.152	30.514		71.45	6
	MOTA	1429	CB	GLU			12.725	55.255	29.664		72.36	6
	MOTA	1430	CG	GLU			13.598	56.429	30.022		40.00	6
	MOTA	1431	CD	GLU			14.875	56.472	29.239		40.00	6
	MOTA	1432	OE1	GLU			15.155	55.565	28.414		40.00	8
15	ATOM	1433	OE2	GLU			15.663	57.430	29.430	1.00		8
	ATOM	1434	С	GLU			10.724	53.912	30.049	1.00		6
	MOTA	1435	0	GLU			10.536	53.701	28.844	1.00	73.02	8
	ATOM	1436	N	CYS			10.301	53.099	30.999	1.00	71.12	7
	MOTA	1437	CA	CYS	Α	446	9.628	51.899	30.634	1.00	70.83	6
20	MOTA	1438	CB	CYS			10.595	50.719	30.687	1.00	71.05	6
	MOTA	1439	SG	CYS			12.009	50.842	29.573	1.00	72.83	16
	MOTA	1440	С	CYS	Α	446	8.454	51.671	31.535	1.00	71.91	6
	MOTA	1441	0	CYS	Α	446	8.495	52.014	32.728	1.00	72.06	8
	MOTA	1442	N	PRO	Α	447	7.372	51.133	30.978	1.00	73.12	7
25	MOTA	1443	CD	PRO			7.267	50.764	29.560	1.00	72.88	6
	MOTA	1444	CA	PRO	Α	447	6.150	50.853	31.740		74.22	6
	MOTA	1445	CB			447	5.187	50.281	30.714	1.00	72.98	6
	MOTA	1446	CG			447	5.875	50.271	29.437	1.00		6
	MOTA	1447	С			447	6.435	49.843	32.831	1.00		6
30	MOTA	1448	0			447	7.181	48.908	32.612	1.00	76.67	8
	MOTA	1449	N			448	5.820	50.002	33.997		76.91	7
	MOTA	1450	CA			448	6.024	49.066	35.113		78.24	6
	ATOM	1451	CB			448	5.528	49.734	36.401	1.00		6
	ATOM	1452	OG1			448	4.105	49.917	36.328	1.00		8
35	ATOM	1453	CG2	THR			6.192	51.081	36.585	1.00		6
	MOTA	1454	С			448	5.113	47.912	34.755		77.42	6
	ATOM	1455	0			448	4.915	46.995	35.519	1.00		8
	ATOM	1456	N			449	4.539	48.021	33.565		76.29	7
40	MOTA	1457	CA			449	3.630	47.023	33.024		75.03	6
40	MOTA	1458	CB			449	2.600	47.773	32.191		74.62	6
	MOTA	1459	CG			449	2.145	47.051	31.001	1.00		6
	MOTA	1460	CD			449	1.297	47.889	30.178			6
	MOTA	1461		GLU			1.479	49.137	30.146	1.00		8
15	ATOM	1462		GLU			0.424		29.497	1.00		8
45	ATOM	1463	C			449	4.434	46.036	32.179	1.00		6
·	ATOM	1464	0			449	3.882	45.142	31.559	1.00		8
	MOTA	1465	N			450	5.747	46.224	32.161	1.00		7
	ATOM	1466	CA			450	6.608	45.347	31.378	1.00		6
50	ATOM	1467	CB			450	7.301	46.154	30.277	1.00		6
50	ATOM	1468	CG			450	6.464	46.819	29.217	1.00		6
	ATOM	1469		LEU			7.337	47.662	28.328	1.00		6
	MOTA	1470		LEU			5.786	45.750	28.415	1.00		6
	ATOM	1471	C			450	7.669	44.673	32.243	1.00		6
<i>E E</i>	ATOM	1472	0			450	8.427	43.841	31.752	1.00		8
55	ATOM	1473	N			451	7.705	45.039	33.530	1.00		7
	ATOM	1474	CA			451	8.681	44.506	34.480	1.00		6
	ATOM	1475	CB			451	9.041	45.562	35.540	1.00		6
	ATOM	1476	CG	PHE	A	451	9.873	46.717	35.008	1.00	63.02	6

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5	ATOM	1477	CD1	PHE A	451	9.426	47.507		1.00 62.92	6 6
,	ATOM	1478		PHE A		11.089	47.017		1.00 63.07 1.00 65.12	6
	ATOM	1479		PHE A		10.199	48.598			6
	ATOM	1480		PHE A		11.860	48.102	35.156	1.00 64.66	6
	ATOM	1481	CZ	PHE A	451	11.410	48.897	34.118	1.00 67.12	6
10	ATOM	1482		PHE A		8.259	43.264	35.260	1.00 56.41	
10	ATOM	1483		PHE A		7.641	43.392	36.331	1.00 56.56	8
		1484		PRO A		8.555	42.045	34.755	1.00 53.28	7
	MOTA	1485	CD	PRO A		9.177	41.689	33.481	1.00 50.46	6
	MOTA	1486	CA	PRO A		8.153	40.859	35.543	1.00 50.26	6
1.5	MOTA	1487	CB	PRO A		8.739	39.680	34.780	1.00 49.19	6
15	MOTA	1488	CG	PRO A		9.178	40.206	33.482	1.00 45.89	6
	ATOM	1489	C	PRO A		8.770	40.999	36.935	1.00 49.62	6
	ATOM		0	PRO A		9.867	41.529	37.094	1.00 52.35	8
	MOTA	1490	Ŋ	PRO A		8.139	40.425	37.947	1.00 51.50	7
	MOTA	1491		PRO A		7.001	39.542	37.797	1.00 49.66	6
20	MOTA	1492	CD	PRO A		8.610	40.528	39.323	1.00 50.89	6
	MOTA	1493	CA	PRO A		7.675	39.659	40.109	1.00 51.49	6
	MOTA	1494	CB	PRO A		6.703	39.141	39.185	1.00 50.82	6
	ATOM	1495	CG	PRO A		10.015	40.084	39.532	1.00 50.99	6
	MOTA	1496	C			10.876	40.900	39.838	1.00 54.17	8
25	ATOM	1497	0	PRO P		10.255	38.781	39.423	1.00 51.21	7
	MOTA	1498	N	LEU A		11.585	38.298	39.674	1.00 47.17	6
	MOTA	1499	CA	LEU A		11.813	36.962		1.00 44.44	6
	MOTA	1500	CB		A 454	13.167	36.375		1.00 41.33	6
	MOTA	1501	CG		A 454	13.524	36.638		1.00 35.93	6
30	MOTA	1502			A 454	13.169			1.00 34.79	6
	MOTA	1503		LEU 2		12.541			1.00 42.25	
	MOTA	1504			A 454	13.477			1.00 40.82	
	MOTA	1505			A 454	12.270			1.00 39.29	
	MOTA	1506			A 455				1.00 41.81	
35	MOTA	1507			A 455	13.133			1.00 47.22	
	ATOM	1508			A 455	12.527				
	MOTA	1509			A 455	13.433				
	MOTA	1510			A 455	14.715				
	MOTA	1511		2 PHE		12.999				
40	MOTA	1512			A 455	15.557				
	MOTA	1513		2 PHE	A 455	13.848				
	MOTA	151	4 CZ	PHE	A 455	15.129				
	MOTA	151	5 C		A 455	13.27				
	ATOM	151	6 0		A 455	14.36				
45	ATOM	151	7 N		A 456	12.15	-			
	ATOM	151			A 456	12.12				
	ATOM		9 CE		A 456	10.68				
	MOTA	152	0 00		A 456	10.06		_	_	
	ATOM	152			A 456	8.59				
50			2 CI		A 456	10.80		_	_	
	ATOM		3 C		A 456	12.73				
	ATON			LEU	A 456	13.59				
	ATO			GLU	A 457	11.97				
	OTA				A 457	12.47				
5	5 ATO				A 457	14.00			· .	
,	ATO				A 457	14.58				
	ATO				A 457	12.02				
	ATO				J A 457	11.11	14 39.4	76 44.42	7 1.00 20.0	,, 6
	AT O									

						10 007	37.994	MOG	14:00-20:00	6
5	MOTA	1531		GLU A		10.807		44.311	1.00 20.00	8
	MOTA	1532		GLU A		11.673	37.099		1.00 20.00	8
	MOTA	1533		GLU A		9.683	37.639	45.172	1.00 23.00	7
	MOTA	1534		VAL A		14.928	41.078	41.903	1.00 44.98	6
	MOTA	1535		VAL A		16.412	41.094	41.868		6
10	MOTA	1536		VAL A		16.881	40.306	40.642	1.00 44.83	6
	MOTA	1537		VAL A		18.365	40.106	40.698	1.00 49.72	
	MCTA	1538		VAL A		16.185	38.979	40.558	1.00 40.89	6
	MOTA	1539		VAL A		17.130	42.420	41.877	1.00 42.72	6
	MOTA	1540	0	VAL A		18.061	42.617	42.658	1.00 42.88	8 7
15	MOTA	1541	N	PHE A		16.713	43.325	41.010	1.00 44.53	
	ATOM'	1542	CA	PHE A		17.385	44.606	40.892	1.00 48.18	6
	ATOM	1543	CB	PHE A		17.281	45.104	39.494	1.00 43.60	6
	MOTA	1544	CG	PHE A		17.915	44.190	38.547	1.00 40.79	6
	MOTA	1545				17.325	42.983	38.244	1.00 41.01	6
20	ATOM	1546	CD2	PHE A	459	19.153	44.483	38.054	1.00 39.48	6
	MOTA	1547	CE1	PHE A		17.988	42.081	37.441	1.00 40.62	6
	MOTA	1548	CE2	PHE A		19.814	43.589	37.257	1.00 36.87	6
	MOTA	1549	CZ	PHE A	459	19.233	42.385	36.940	1.00 36.39	6
	MOTA	1550	С	PHE A		16.837	45.648	41.744	1.00 52.71	6
25	MOTA	1551	0	PHE A		17.492	46.682	42.017	1.00 51.34	8
	MOTA	1552	N	GLU A	460	15.606	45.422	42.161	1.00 62.92	7
	MOTA	1553	CA	GLU A	460	15.066	46.428	42.965	1.00 69.33	6
	MOTA	1554	CB	GLU P		13.552	46.352	43.094	1.00 72.95	6
	MOTA	1555	CG	GLU A		12.978	47.767	42.957	1.00 78.35	6
30	ATOM	1556	CD	GLU A		12.246	48.261	44.157	1.00 82.97	6
	MOTA	1557	OEl	GLU A		12.471	47.759	45.281	1.00 88.28	8
	MOTA	1558	OE2	GLU A		11.422	49.200	44.017	1.00 84.80	8
	MOTA	1559	С	GLU A		15.736	46.245	44.272		6
	MOTA	1560	0	GLU A		16.187	45.170	44.691		8
35	MOTA	1561	N	ASP A		15.790	47.373	44.917		7
	MOTA	1562	CA	ASP A		16.415	47.505	46.173		6
	ATOM	1563	CB		4 461	16.394	48.981	46.471		6 6
	MOTA	1564	CG		A 461	16.801	49.786	45.276		8
	ATOM	1565		ASP 2		16.692	49.344	44.086		8
40	MOTA	1566		ASP :		17.239	50.923	45.482		6
	MOTA	1567	С		A 461	15.639	46.703	47.214		8
	MOTA	1568	0		A 461	16.245	45.748	47.731		8
	MOTA	1569	OXI	ASP .	A 461	14.457	47.026	47.45]	1.00 88.70	0
	TER					22 222	66 051	20 797	1.00 46.72	6
45	ATOM	1			B 211	-20.802		39.780		6
	MOTA	2			B 211	-19.566		39.922		6
	MOTA	3			B 211	-18.264		40.045		6
	ATOM	4			B 211	-18.043		38.886		7
	MOTA	5			B 211	-19.008		38.903		6
50	MOTA	6			B 211	-22.418		40.818		8
	MOTA	7			B 211	-23.356		40.45		7
	MOTA	8			B 211	-20.742		42.239		6
	MOTA	9			B 211	-20.998		40.89		7
	MOTA	10			B 212	-22.610		41.06		6
55	ATOM	11			B 212	-21.526		41.28		6
	ATOM	12			B 212	-23.943		41.03		6
	MOTA	13			B 212	-23.657		41.42		6
	ATOM	14	CG	PRO	B 212	-22.226	71.474	41.55	1.00 42.00	J

5	ATOM	15		PRO B 212		-24.798		39.807	1.00 38		6
	MOTA	16		PRO B 212		-24.350	70.045	38.696	1.00 34		8
	MOTA	17	N G	LU B 213	3	-26.058	69.424	40.032	1.00 40		7
	ATOM	18	CA C	LU B 213	3	-27.081	69.290	39.003	1.00 43		6
	MOTA	19	CB G	LU B 213	3	-27.895	68.004	39.265	1.00 45		6
10	ATOM	20	CG (SLU B 213	3	-27.032	66.709	39.286	1.00 4		6
	ATOM	21	CD (GLU B 21	3	-27.807	65.421	39.199	1.00 5		6
	MOTA	22	OE1 (GLU B 21	3	-28.847	65.244	39.886	1.00 5		8
	ATOM	23	OE2	GLU B 21	3	-27.382	64.516	38.442	1.00 4		8
	ATOM	24	C (GLU B 21	3	-27.924	70.576	39.080	1.00 4		6
15	ATOM	25		GLU B 21	3	-27.624	71.467	39.859	1.00 4		8
	ATOM	26	N	PRO B 21	4	-28.987	70.698	38.308	1.00 4		7
	MOTA	27	CD	PRO B 21	4	-29.484	69.635	37.446	1.00 4		6
	ATOM	28		PRO B 21	4	-29.843	71.907	38.302	1.00 4		6
	ATOM	29		PRO B 21	.4	-30.799	71.639	37.210	1.00 4		6
20	ATOM	30	CG	PRO B 21	. 4	-30.530	70.257	36.805	1.00 4		6
20	ATOM	31	C	PRO B 21	. 4	-30.574	72.330	39.535	1.00 4	5.70	6
	ATOM	32		PRO B 21		-30.597	71.595	40.483	1.00 4		8
	ATOM	33		THR B 21	.5	-31.180	73.515	39.506	1.00 4		7
	ATOM	34		THR B 21	15	-31.965	74.036	40.652	1.00 4		6
25	MOTA	35		THR B 21		-31.443	75.420	41.091	1.00 4		6
_3	ATOM	36		THR B 21		-32.249	76.464	40.534	1.00 5		8
	ATOM	37	_	THR B 21		-30.011	75.617	40.659	1.00 3		6
	ATOM	38	С	THR B 23		-33.386	74.239	40.114	1.00 5		6
	ATOM	39	0	THR B 23		-33.562	74.868	39.078	1.00 5		8
30	ATOM	40	N	ASP B 2		-34.387	73.741	40.829	1.00 5		7
50	MOTA	41	CA	ASP B 2		-35.795	73.865	40.435		51.51	6
	MOTA	42	CB	ASP B 2		-36.674	74.005	41.650		70.57	6
	ATOM	43	CG	ASP B 2		-37.675	72.981	41.710		78.07	6
	MOTA	44	OD1	ASP B 2	16	-38.228	72.588	40.652	1.00 8		8
35	MOTA	45	OD2	ASP B 2	16	-37.983	72.567	42.830	1.00		8
• -	MOTA	46	С	ASP B 2	16	-35.920	75.123	39.648	1.00		6
	ATOM	47	0	ASP B 2	16	-36.847	75.317	38.827	1.00		8
	ATOM	48	N	GLU B 2	17	-34.954	75.979	39.984	1.00		7
	MOTA	49	CA	GLU B 2	17	-34.851	77.259	39.353	1.00		6
40	MOTA	50	CB	GLU B 2	17	-34.104	78.264	40.251		51.02	6
	MOTA	51	CG	GLU B 2		-34.151	79.689	39.679	1.00		6
	MOTA	52	CD	GLU B 2	17	-34.301	80.745	40.739	1.00		6
	MOTA	53	OE1	GLU B 2	17	-34.089	80.443	41.945	1.00		8
	MOTA	54	OE2	GLU B 2	17	-34.625		40.411	1.00		8
45	MOTA	55	C	GLU B 2	17	-34.232		37.957	1.00		6
	ATOM	5€	0	GLU B 2	217	-34.815		37.018	1.00		8
	MOTA	57	N	GLU B 2		-33.063		37.839		49.20	7
	ATOM	58	CA	GLU B 2	218	-32.318		36.608		45.94	6
	MOTA	59	CB	GLU B 2	218	-30.965		36.981		43.43	6
50		60) CG	GLU B 2	218	-30.065		37.801		40.86	6
	ATOM	61	CD	GLU B 2	218	-28.713				39.88	6
	MOTA	62		GLU B 2		-28.606				37.61	8
	ATOM	63	OE2	GLU B 2	218	-27.707	76.901			34.01	8
	ATOM	64		GLU B 2		-33.014				44.71	6
55		6.5		GLU B 2		-32.935				45.31	8
	ATOM	6		TRP B 2		-33.669				44.02	7
	ATOM	6		TRP B 2		-34.368				46.97	6
	ATOM	6		TRP B		-35.046	72.408	36.119	1.00	48.42	6
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5	ATOM	69		TRP B		-34.195	71.230	36.374	1.00 54.61	6
	ATOM	70		TRP B		-34.048	70.120	35.478	1.00 55.24	6
	MOTA	71		TRP B		-33.076	69.248	36.063	1.00 53.67	6
	ATOM	72		TRP B		-34.615	69.771	34.252	1.00 54.55	6
	MOTA	73		TRP B		-33.399	71.019	37.415	1.00 55.75	6
10	ATOM	74	NE1	TRP B	219	-32.697	69.838	37.236	1.00 54.43	7
	ATOM	75	CZ2	TRP B	219	-32.635	68.075	35.431	1.00 52.54	6
	ATOM	76	CZ3	TRP B	219	-34.214	68.603	33.643	1.00 55.17	6
	MOTA	77	CH2	TRP B	219	-33.234	67.758	34.214	1.00 55.59	6
	ATOM	78	C	TRP B	219	-35.409	74.199	34.459	1.00 47.32	6
15	ATOM	79	0	TRP B	219	-35.561	73.914	33.277	1.00 43.56	8
	ATOM	80	N	GLU B	220	-36.126	75.130	35.084	1.00 49.91	7
	MOTA	81	CA	GLU B	220	-37.158	75.874	34.402	1.00 53.57	6
	ATOM	82	CB	GLU B	220	-37.811	76.820	35.373	1.00 58.18	6
	ATOM	83	CG	GLU B	220	-39.251	76.812	35.221	1.00 73.13	6
20	ATOM	84	CD	GLU B	220	-39.824	76.858	36.489	1.00 80.06	6
	ATOM	85	OE1	GLU B	220	-39.485	75.995	37.324	1.00 82.12	8
	ATOM	86	OE2	GLU B		-40.635	77.740	36.718	1.00 82.78	8
	ATOM	87	С	GLU B		-36.539	76.645	33.250	1.00 50.51	6
	ATOM	88	0	GLU B		-37.160	76.793	32.195	1.00 49.94	8
25	ATOM	89	N	LEU B		-35.312	77.135	33.455	1.00 43.71	7
	ATOM	90	CA	LEU E		-34.604	77.884	32.411	1.00 42.81	6
	ATOM	91	СВ	LEU E		-33.214	78.324	32.865	1.00 39.21	6
	ATOM	92	CG	LEU E		-32.321	78.833	31.754	1.00 36.34	6
	ATOM	93	CD1	LEU E		-33.073	79.843	30.927	1.00 36.93	6
30	ATOM	94	CD2	LEU E		-31.058	79.446	32.331	1.00 24.18	6
	ATOM	95	С	LEU E		-34.454	77.011	31.192	1.00 43.46	6
	ATOM	96	0	LEU E		-34.819	77.406	30.104	1.00 45.25	8
	MOTA	97	N	ILE E	3 222	-33.878	75.829	31.398	1.00 39.09	7
	MOTA	98	CA	ILE E	3 222	-33.687	74.857	30.330	1.00 35.47	6
35	ATOM	99	CB	ILE E	3 222	-33.224	73.516	30.871	1.00 33.74	6
	MOTA	100	CG2	ILE E	3 222	-33.204	72.488	29.776	1.00 28.86	6
	MOTA	101	CG1	ILE E	3 222	-31.840	73.631	31.493	1.00 33.33	6
	MOTA	102	CD1	ILE H	3 222	-31.435	72.419	32.264	1.00 34.85	6
	ATOM	103	С	ILE H	3 222	-34.991	74.627	29.598	1.00 34.26	6
40	ATOM	104	0	ILE E	3 222	-35.082	74.832	28.392	1.00 31.90	8
	MOTA	105	N	LYS I	3 223	-35.992	74.183	30.346	1.00 39.49	7
	ATOM	106	CA	LYS I	3 223	-37.300	73.892	29.785	1.00 44.43	6
	MOTA	107	CB	LYS I	3 223	-38.351	73.876	30.882	1.00 50.81	6
	ATOM	108	CG	LYS I	3 223	-39.693	73.358	30.411	1.00 62.51	6
45	MOTA	109	CD	LYS I	B 223	-40.795	73.532	31.449	1.00 72.22	6
	MOTA	110	CE	LYS 1	B 223	-42.163	73.249	30.827	1.00 74.55	6
	ATOM	111	NZ	LYS 1	B 223	-43.268	73.378	31.837	1.00 75.78	7
	MOTA	112	С	LYS :	B 223	-37.648	74.942	28.755	1.00 42.81	6
	ATOM	113	0	LYS :	B 223	-38.337	74.661	27.796	1.00 40.36	8
50	MOTA	114	N	THR	В 224	-37.146	76.156	28.979	1.00 39.89	7
	MOTA	115	CA	THR	B 224	-37.353	77.293	28.074	1.00 39.93	6
	MOTA	116	CB	THR	B 224	-36.956	78.609	28.776		6
	MOTA	117	OG1	THR	в 224	-37.646	78.740	30.028	1.00 39.27	8
	ATOM	118		THR			79.805	27.893		6
55	ATOM	119			B 224		77.094	26.789		6
	ATOM	120	0		B 224		76.677	25.756	1.00 36.67	8
	ATOM	121	N		B 225		77.421	26.888		7
	ATOM	122			B 225		77.295	25.801	1.00 38.12	6

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5	ATOM	123	CB V	AL B 22	5	-32.869	77.015	28.346	1600	B. 2 93 3	<u></u>
3	ATOM		CG1 V			-31.863	76.983	25.226	1.00 3		6
			CG2 V			-32.483	78.050	27.353	1.00 4		6
	MOTA			AL B 22		-34.656	76.191	24.843	1.00 3	37.52	6
	MOTA	127		AL B 22		-34.621	76.364	23.638	1.00 3	36.77	8
10	ATOM			HR B 22		-35.005	75.046	25.410	1.00 3	34.02	7
10	ATOM	128		HR B 22		-35.423	73.887	24.638	1.00 3	34.67	6
	ATOM	129		HR B 22		-35.677	72.707	25.574	1.00	30.56	6
	ATOM	130		HR B 22		-34.432	72.225	26.084		32.20	8
	MOTA	131				-36.413	71.595	24.874		20.99	6
	MOTA	132		HR B 22 HR B 22		-36.664	74.170	23.803		36.41	6
15	ATOM	133			26	-36.633	74.054	22.578	1.00	39.64	8
	MOTA	134		LA B 22		-37.746	74.542	24.480	1.00		7
	ATOM	135		LA B 2		-39.008	74.861	23.822		36.93	6
	MOTA	136		LA B 2		-39.914	75.631	24.785		38.06	6
	MOTA	137				-38.686	75.719	22.608		37.69	6
20	MOTA	138			27	-39.317	75.616	21.566		40.94	8
	MOTA	139			27	-37.677	76.572	22.785		32.86	7
	MOTA	140		ALA B 2		-37.216	77.483	21.753		32.48	6
	MOTA	141		ALA B 2		-36.252	78.458	22.358		28.25	6
	MOTA	142			28	-36.232	76.704	20.638		36.12	6
25	MOTA	143		ALA B 2		-37.078	76.586	19.544		37.86	8
	MOTA	144		ALA B 2		-35.364	76.175	20.924		33.58	7
	MOTA	145			29	-34.611	75.409	19.956		32.97	6
	MOTA	146	-		29	-33.418	74.721	20.597		33.69	6
	MOTA	147			229	-32.776	73.714	19.715		28.39	6
30	MOTA	148			229	-32.535	72.384	19.863		28.83	6
	MOTA	149			229	-32.336	74.030	18.426		30.47	7
	MOTA	150			229	-31.867	72.929	17.855		26.95	6
	MOTA	151	CE1		229	-31.976	71.927	18.700		31.27	7
	MOTA	152	NE2		229	-35.362	74.352	19.202		38.40	6
35	MOTA	153			229 229	-35.069	74.332	18.045		41.49	8
	MOTA	154				-36.296	73.688	19.882		38.55	7
	MOTA	155			230	-37.077	72.634	19.263	1.00		6
	MOTA	156			230	-37.744	71.747	20.310		44.68	6
4.0	MOTA	157	CB		230	-38.381		19.637	1.00		6
40	MOTA	158		VAL B		-36.742		21.356		42.18	6
	ATOM	159		VAL B		-38.133				44.28	6
	ATOM ·	160	C	VAL B		-38.375				45.94	8
	ATOM	161	0	ALA B		-38.774				45.59	7
4.5	ATOM	162		ALA B		-39.820				47.84	6
45	MOTA	163		ALA B		-40.736				45.08	6
	MOTA	164				-39.235				48.04	6
	ATOM	165		ALA B		-39.959				49.95	8
	ATOM	166		ALA B		-37.914				47.26	7
	MOTA	167		THR B		-37.220				43.64	6
50		168		THR B		-36.482				41.93	6
	MOTA	169		THR B						39.10	8
	MOTA	170				-35.385				29.80	
	MOTA	171		THR B		-37.423				43.97	
	MOTA	172		THR B		-36.194				40.55	
55		173		THR B		-35.40				48.62	
	MOTA	174		ASN B		-36.19				58.62	
	MOTA	175		ASN B		-35.24				62.44	
	MOTA	176	5 CB	ASN B	233	-34.62	12.55	, 13.500	. 1.50	 -	

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5	ATOM	177	CG	ASN B		-33.407	72.427	14.256	1.00		8
	ATOM	178		ASN B		-32.569	70.529	15.265		74.29	7
	ATOM	179		ASN B		-33.288 -36.033	70.329	13.437		65.06	6
	ATOM	180	С	ASN B			72.733	13.754		69.47	8
	MOTA	181	0	ASN B		-36.950	72.003	12.182		68.80	7
10	ATOM	182	N	ALA B		-35.674	72.376	11.036		70.98	6
	ATOM	183	CA	ALA B		-36.352	72.701	9.769		71.43	6
	ATOM	184	CB	ALA B		-35.585		11.111		73.83	6
	MOTA	185	С	ALA B		-36.556	70.880	11.501		74.33	8
	MOTA	186	0	ALA B		-35.677	70.142			75.07	7
15	MOTA	187	N	GLN B		-37.754	70.479	10.717 10.690	1.00	76.32	6
	ATOM	188	CA	GLN B		-38.149	69.095	9.533	1.00	76.98	6
	ATOM	189	CB	GLN B		-37.468	68.365	8.170	1.00	77.07	6
	MOTA	190	CG	GLN B		-38.120	68.540	7.909	1.00	80.85	6
	MOTA	191	CD	GLN E		-38.572	69.940	8.491	1.00		8
20	MOTA	192	OE1			-39.575	70.401	7.040	1.00	78.80	7
	MOTA	193	NE2			-37.862	70.620		1.00	77.15	6
	MOTA	194	С	GLN F		-37.904	68.331	11.953	1.00	76.06	8
	MOTA	195	0	GLN E		-38.087	67.137	11.947	1.00	77.46	7
	MOTA	196	N	GLY E		-37.511	68.985	13.039 14.288	1.00	78.37	6
25	ATOM	197	CA	GLY E		-37.304	68.263	14.200	1.00	79.43	6
	ATOM	198	С	GLY E		-36.717	66.882 66.650	13.542	1.00	79.47	8
	MOTA	199	0	GLY E		-35.717	66.007	14.943	1.00	77.98	7
	MOTA	200	N		3 237	-37.420	64.600	15.092	1.00	76.49	6
	MOTA	201	CA	SER I		-37.117 -38.118	63.953	16.066	1.00	76.46	6
30	MOTA	202	CB	SER I		-37.181	63.895	13.737	1.00	75.35	6
	MOTA	203	C	SER I		-36.493	62.911	13.737	1.00	75.47	8
	MOTA	204	0	SER I		-38.004	64.443	12.845	1.00	75.56	7
	ATOM	205	N	HIS I		-38.293	63.926	11.519	1.00	75.46	6
25	ATOM	206	CA	HIS I		-39.663	64.397	11.096		75.85	6
35	ATOM	207	CB C	HIS		-37.369	64.216	10.380		74.10	6
	ATOM	208 209	0		B 238	-37.747	64.135	9.222		75.34	8
	MOTA	210	N		B 239	-36.127	64.427	10.651			7
	MOTA MOTA	210	CA		B 239	-35.345	64.786	9.519			6
40	MOTA	211	CB		B 239	-34.121	65.542	9.934			6
40	ATOM	213	CG		B 239	-33.085	64.786	10.737		89.67	6
	MOTA	213	CD:		B 239	-31.727	64.530	10.302		93.19	6
	MOTA	215		2 TRP		-31.069	63.848			95.46	6
	MOTA	216		3 TRP		-30.949	64.941			95.35	6
45	MOTA	217		1 TRP		-33.237	64.180		1.00	94.16	6
73	MOTA	218		1 TRP		-32.022	63.631		1.00	97.48	7
	MOTA	219		2 TRP		-29.706	63.475			96.23	6
	MOTA	220		3 TRP		-29.613	64.533			96.75	6
	ATOM	221		2 TRP		-28.978	63.870		1.00	97.32	6
50	ATOM	222			B 239	-34.994	63.722		1.00	70.77	6
50	ATOM	223			B 239	-35.423			1.00	71.70	8
	MOTA	224			B 240	-34.165				67.10	7
	ATOM	225			в 240	-33.724				65.63	6
	MOTA	226			B 240	-33.321				66.65	6
55	MOTA	227			B 240	-32.210				69.83	6
55	MOTA	228			B 240	-31.759				71.49	6
	MOTA	229			B 240	-30.576				71.31	6
	ATOM	230			B 240	-30.106				72.23	7
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5	ATOM	231	С	LYS B 2		-34.719	61.331	6.996		66; 193	
	ATOM	232	0	LYS B 2		-34.321	60.673	6.031	1.00		8
	MOTA	233	N	ASN B 2		-35.986	61.727	7.139		66.69	7
	MOTA	234	CA	ASN B 2	241	-37.031	61.393	6.171	1.00		6
	MOTA	235	CB		241	-38.240	60.846	6.915	1.00		6
10	MOTA	236	CG	ASN B 2	241	-37.966	59.479	7.544		70.19	6
	ATOM	237	OD1	ASN B 2	241	-37.561	58.526	6.845		71.37	8
	MOTA	238	ND2	ASN B 2	241	-38.205	59.370	8.836		71.48	7
	ATOM	239	С	ASN B 2	241	-37.496	62.532	5.255		66.62	6
	ATOM	240	Ο.	ASN B	241	-38.504	62.395	4.578		64.76	8
15	ATOM	241	N	LYS B	242	-36.753	63.633	5.209		66.86	7
	MOTA	242	CA	LYS B	242	-37.096	64.772	4.362		67.46	6
	ATOM	243	CB	LYS B	242	-37.501	65.948	5.258		67.93	6
	MOTA	244	CG	LYS B	242	-38.746	65.684	6.076		71.52	6
	MOTA	245	CD	LYS B	242	-40.007	65.528	5.215		74.32	6
20	MOTA	246	CE	LYS B	242	-40.416	66.852	4.564	1.00	74.41	6
	MOTA	247	NZ	LYS B	242	-40.657	67.941	5.575		74.44	7
	ATOM	248	С	LYS B	242	-35.826	65.081	3.592		66.28	6
	MOTA	249	0	LYS B	242	-35.814	65.799	2.601	1.00		8
	ATOM	250	N	ARG B	243	-34.763	64.485	4.112	1.00		7
25	ATOM	251	CA	ARG B	243	-33.410	64.577	3.591	1.00		6
	MOTA	252	CB	ARG B	243	-32.599	63.547	4.390	1.00	60.12	6
	MOTA	253	CG	ARG B	243	-31.128	63.558	4.171	1.00	40.00	6
	MOTA	254	CD	ARG B	243	-30.335	62.888	5.319	1.00	40.00	6
	ATOM	255	NE	ARG B	243	-30.269	61.428	5.296	1.00	40.00	7
30	MOTA	256	CZ	ARG B	243	-29.384	60.724	6.009	1.00	40.00	6
	MOTA	257	NH1	ARG B	243	-28.510	61.357	6.798	1.00	40.00	7
	MOTA	258	NH2			-29.355	59.401	5.908	1.00	40.00	7
	MOTA	259	С	ARG B		-33.408	64.252	2.100		62.97	6
	MOTA	260	0	ARG B		-33.690	63.122	1.722		63.96	8
35	MOTA	261	N	LYS B		-33.105	65.245	1.270		62.41	7
	MOTA	262	CA	LYS B		-33.054	65.053	-0.179	1.00		6
	MOTA	263	CB		244	-34.104	65.941	-0.866		63.68	6
	MOTA	264	CG	LYS B		-35.527	65.731	-0.337	1.00		6
	MOTA	265	CD	LYS B	244	-36.566	66.549	-1.107	1.00	73.83	6
40	MOTA	266	CE	_	244	-36.219	68.045	-1.138	1.00		6 7
	ATOM	267	NZ	LYS B		-36.169	68.689	0.219	1.00	73.32	
	MOTA	268	С	LYS B		-31.658		-0.670	1.00		6
	MOTA	269	0	LYS B		-31.317		-0.852		56.34	8
	MOTA	270	N	PHE B		-30.858		-0.875		57.06	7
45	MOTA	271	CA	PHE B		-29.462		-1.305		59.01	6
	MOTA	272		PHE B		-28.786		-1.478		59.62	6
	MOTA	273		PHE B		-28.991		-0.339		66.60	6
	MOTA	274		1 PHE B		-30.200		-0.172		67.17	6
	MOTA	275		2 PHE B		-28.012		0.593		69.25	6
50	MOTA	276	CE	1 PHE B		-30.404		0.911		69.92	6
	ATOM	277	CE	2 PHE B	245	-28.229		1.669		70.50	6
	MOTA	278	CZ			-29.418		1.830			6
	ATOM	279	C	PHE B		-29.301		-2.592		60.68	6
	MOTA	280	0	PHE B		-29.859		-3.619		62.37	
55	ATOM	281	. N	LEU B		-28.495		-2.505		60.10	
	ATOM	282	CA			-28.201		-3.631		59.44	
	MOTA	283	CB			-27.248		-3.231		57.43	
	ATOM	284	CG	LEU B	246	-27.118	69.474	-4.207	1.00	54.41	6

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5	ATOM	285		LEU B		-28.481		-3.719	1.00 52.45	6
	MOTA	286			246	-26.112	70.470	-4.740	1.00 51.05	6
	MOTA	287		LEU B		-27.585	66.379		1.00 52.05	8
	ATOM	288		LEU B		-26.789	65.446	-4.486		7
	MOTA	289	N	PRO B	247	-27.930	66.693	-5.984	1.00 63.33	
10	MOTA	290	CD	PRO B	247	-28.839	67.781	-6.363	1.00 64.44	6
	MOTA	291	CA	PRO B		-27.391	65.958	-7.130	1.00 63.56	6
	ATOM	292	CB	PRO B		-27.976	66.675	-8.340	1.00 64.42	6
	ATOM	293	CG	PRO B	247	-28.873	67.714	-7.841	1.00 64.90	6
	ATOM	294	С	PRO B	247	-25.866	65.947	-7.143	1.00 61.94	6
15	MOTA	295	0	PRO B	247	-25.223	66.944	-6.856	1.00 61.60	8
	MOTA	296	N	GLU B	248	-25.333	64.771	-7.478	1.00 61.33	7
	MOTA	297	CA	GLU B	248	-23.896	64.516	-7.590	1.00 63.50	6
	MOTA	298	CB	GLU B	248	-23.630	63.154	-8.248	1.00 66.94	6
	ATOM	299	CG	GLU B	248	-22.168	62.953	-8.713	1.00 68.70	6
20	ATOM ·	300	CD	GLU B		-21.898	61.745	-9.580	1.00 40.00	6
20	ATOM	301	OE1	GLU B		-22.863		-10.035	1.00 40.00	8
	ATOM	302	OE2	GLU B		-20.709	61.460	-9.838	1.00 40.00	8
	MOTA	303	C	GLU B		-23.158	65.571	-8.415	1.00 64.19	6
	ATOM	304	0	GLU B		-22.056	65.975	-8.066	1.00 65.56	8
25	ATOM	305	N	ASP B		-23.796	66.019	-9.498	1.00 64.36	7
23	ATOM	306	CA	ASP B		-23.254		-10.436	1.00 63.33	6
	ATOM	307	CB	ASP B		-24.122		-11.698	1.00 62.97	6
	MOTA	308	CG	ASP E		-25.437		-11.489	1.00 64.63	6
	MOTA	309		ASP E		-26.235		-10.629	1.00 64.84	8
20		310		ASP E		-25.726		-12.189	1.00 66.52	8
30	MOTA	310	C	ASP E		-23.068	68.413	-9.960	1.00 64.31	6
	MOTA	311	0	ASP E		-22.117		-10.355	1.00 64.73	8
	ATOM	312	N	ILE E		-23.987	68.892	-9.136	1.00 63.09	7
	MOTA	314	CA	ILE E		-23.921	70.281	-8.660	1.00 64.39	6
25	MOTA	314	CB	ILE E		-25.124	70.575	-7.798	1.00 65.79	6
35	ATOM		CG2			-25.559	72.041	-7.858	1.00 64.78	6
	MOTA	316				-26.348	69.752	-8.206	1.00 65.28	6
	ATOM	317	CG1			-27.671	70.444	-7.887	1.00 65.08	6
	ATOM	318	CD1	ILE H		-22.815	70.488	-7.714	1.00 65.21	6
40	ATOM	319	С		3 250	-22.754	69.847	-6.656	1.00 64.05	8
40	MOTA	320	0			-22.024	71.392	-8.103	1.00 65.48	7
	MOTA	321	N	GLY I		-20.873	71.721	-7.342	1.00 67.32	6
	MOTA	322	CA		3 251	-19.808	70.806	-7.800	1.00 68.52	6
	ATOM	323	C		3 251			-9.025	1.00 65.49	8
	ATOM	324	0		3 251	-19.791		-6.799	1.00 72.26	7
45	MOTA	325	N		3 252	-19.074		-6.883	1.00 72.20	6
	MOTA	326	CA		3 252	-17.949			1.00 75.82	6
	ATOM	327	CB		B 252	-18.460		-6.723		
	MOTA	328	CG		B 252	-17.367		-6.356	1.00 77.81	6
	ATOM	329	CD		B 252	-17.924		-5.824	1.00 79.38	6
50	MOTA	330		GLN		-18.615		-6.549		8
	MOTA	331		GLN		-17.661				7
	MOTA	332			B 252	-17.258				6
	MOTA	333			B 252	-17.977				8
	MOTA	334			в 253	-15.718				7
55	ATOM	335	CA		в 253	-14.615				6
	MOTA	336	СВ		в 253	-13.794				6
	MOTA	337	С	ALA	B 253	-13.605				6
	MOTA	338	0	ALA	в 253	-13.186	69.691	-10.171	1.00 85.69	8

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5	ATOM	339	N	PRO B 254	-13.223				10 PJ 3.	
	MOTA	340	CD	PRO B 254	-13.798	73.217	-9.752	1.00 3		6
	ATOM	341	CA	PRO B 254	-12.266	72.177 -		1.00 3		6
	ATOM	342	CB	PRO B 254	-12.275	73.710 -		1.00 3		6
	MOTA	343	CG	PRO B 254	-13.222	74.277 -		1.00 3		6
10	ATOM	344	С	PRO B 254	-10.827	71.665 -		1.00		6
	MOTA	345	0	PRO B 254	-10.379	71.426	-10.009	1.00	38.78	8
	TER									-
	ATOM	1	N	GLY B 261	-8.238	79.356	-2.979	1.00		7
	MOTA	2	CA	GLY B 261	-9.314	78.411	-3.005	1.00		6
15	ATOM	3	С	GLY B 261	-10.206	78.717	-4.355	1.00		6
	ATOM	4	0	GLY B 261	-11.372	79.141	-4.256	1.00		8
	ATOM	5	N	GLY B 262	-9.565	78.527	-5.597	1.00		7
	MOTA	6	CA	GLY B 262	-10.136	78.609	-7.087	1.00		6
	MOTA	7	С	GLY B 262	-10.849	79.966	-7.577	1.00		6
20	MOTA	8	0	GLY B 262	-10.200	81.044	-7.543	1.00		8
	MOTA	9	N	LYS B 263	-12.086	79.687	-8.124		61.71	7
	ATOM	10	CA	LYS B 263	-13.323	80.536	-8.428		64.36	6
	MOTA	11	С	LYS B 263	-14.367	79.750	-7.614		63.41	6
	MOTA	12	0	LYS B 263	-14.102	78.579	-7.280		61.93	8 6
25	MOTA	13	CB	LYS B 263	-13.901	80.405	-9.876		63.50	6
	MOTA	14	CG	LYS B 263	-13.487		-10.881		20.00	6
	MOTA	15	CD	LYS B 263	-14.016		-10.612		20.00	6
	MOTA	16	CE	LYS B 263	-13.641		-11.742		20.00	7
	ATOM	17	NZ	LYS B 263	-13.680		-11.341		61.15	7
30	MOTA	18	И	VAL B 264	-15.489		-7.307		59.46	6
	MOTA	19	CA	VAL B 264	-16.616		-6.619 -6.099		59.40	6
	MOTA	20	CB	VAL B 264	-17.574		-6.099 -4.979		53.79	6
	MOTA	21	CG:		-18.479		-5.562		55.32	6
	ATOM	22	CG2		-16.847		-7.700		60.96	6
35	MOTA	23	С	VAL B 264	-17.330		-8.873		62.13	8
	MOTA	24	0	VAL B 264	-16.940		-7.340		62.59	7
	MOTA	25	N	ASP B 265	-18.378 -19.175		-8.312		64.95	6
	MOTA	26	CA	ASP B 265	-18.796		-8.270		64.32	6
4.0	MOTA	27	CB	ASP B 265	-19.928		-8.584		67.70	6
40	MOTA	28	CG	ASP B 265 1 ASP B 265	-20.856		-9.295		72.59	8
	MOTA	29		2 ASP B 265	-20.370					8
	ATOM	30		ASP B 265	-20.658				65.64	6
	ATOM	31	C	ASP B 265	-21.342				68.81	8
4 ~	MOTA	32		LEU B 266	-21.066				65.12	7
45	ATOM	33 34			-22.38				63.40	6
	MOTA	35			-22.429				67.34	6
	MOTA	36			-21.29				69.35	6
	MOTA	37		1 LEU B 266					68.24	6
50	MOTA	38		2 LEU B 266					70.47	6
50		39		LEU B 266					59.67	6
	MOTA	40		LEU B 266					53.35	8
	ATOM	41		GLU B 267					58.01	7
	MOTA	42							58.34	6
55	MOTA	4.2					-10.368		59.21	6
33		43					-10.268		62.89	6
	ATOM	45					-11.328	1.00	67.66	6
	MOTA	46		E1 GLU B 267			-11.512		69.95	8
	MOTA	4.6	. 01	11 010 1 20,		_				

					6	12:-008	4:00 69.40	^
5	ATOM	47 OE2		-27.098				
	ATOM	48 C	GLU B 267	-25.200		-8.032	1.00 57.67	6
	MOTA	49 O	GLU B 267	-26.354		-7.643	1.00 58.34	8
	MOTA	50 ท	ALA B 268	-24.114		-7.285	1.00 53.43	7
	MOTA	51 CA	ALA B 268	-24.151		-5.905	1.00 49.00	6
10	ATOM	52 CB	ALA B 268	-22.816		-5.526	1.00 45.72	6
	MOTA	53 C	ALA B 268	-24.421		-5.056	1.00 45.76	6
	ATOM	54 O	ALA B 268	-25.419	76.823	-4.351	1.00 41.50	8
	ATOM	55 N	PHE B 269	-23.533	77.766	-5.142	1.00 41.43	7
	ATOM	56 CA	PHE B 269	-23.688	78.989	-4.358	1.00 43.96	6
15	ATOM	57 CB	PHE B 269	-22.903	80.150	-4.971	1.00 40.10	6
	ATOM	58 CG	PHE B 269	-23.057	81.458 [.]	-4.224	1.00 40.44	6
	MOTA	59 CD	1 PHE B 269	-22.284	81.727	-3.105	1.00 38.98	6
	ATOM	60 CD	2 PHE B 269	-24.033	82.372	-4.603	1.00 37.15	6
	ATOM	61 CE		-22.472	82.921	-2.388	1.00 32.12	6
20	ATOM	62 CE		-24.228	83.567	-3.890	1.00 38.41	6
	ATOM	63 CZ		-23.457	83.838	-2.780	1.00 40.55	6
	MOTA	64 C	PHE B 269	-25.154	79.374	-4.320	1.00 49.76	6
	ATOM	65 0	PHE B 269	-25.645	79.905	-3.336	1.00 52.15	8
	ATOM	66 N	SER B 270	-25.840 ·	79.112	-5.426	1.00 53.15	7
25	MOTA	67 CA		-27.253	79.431	-5.520	1.00 52.29	6
23	ATOM	68 CE		-27.742	79.274	-6.948	1.00 51.85	6
	ATOM	69 00		-29.118	79.606	-7.048	1.00 53.42	8
	ATOM	70 C	SER B 270	-28.012	78.486	-4.630	1.00 49.38	6
	MOTA	71 0	SER B 270	-28.438	78.864	-3.548	1.00 48.74	8
30	MOTA	72 N	HIS B 271	-28.185	77.253	-5.115	1.00 50.15	7
30	MOTA	73 CF		-28.904	76.203	-4.382	1.00 51.67	6
	MOTA	74 CE		-28.409	74.812	-4.782	1.00 58.52	6
	ATOM	75 CC		-29.096	74.248	-5.976	1.00 68.97	6
	ATOM		02 HIS B 271	-29.987	73.233	-6.102	1.00 70.88	6
35	ATOM		D1 HIS B 271	-28.943	74.770	-7.270	1.00 71.98	7
55	ATOM		E1 HIS B 271	-29.716	74.080	-8.100	1.00 73.91	6
	ATOM		E2 HIS B 271	-30.354	73.149	-7.419	1.00 73.59	7
	ATOM	80 C	HIS B 271	-28.785	76.347	-2.886	1.00 48.33	6
	MOTA	81 0	HIS B 271	-29.641	75.874	-2.156	1.00 48.39	8
40	MOTA	82 N		-27.702	76.992	-2.444	1.00 41.34	7
	ATOM	83 C	A PHE B 272	-27.440	77.224	-1.033	1.00 39.44	6
	MOTA	84 C	B PHE B 272	-25.936	77.302	-0.801	1.00 36.67	6
	ATOM	85 C		-25.241	75.945	-0.861	1.00 33.39	6
	ATOM		D1 PHE B 272	-23.856	75.857	-0.976		6
45	MOTA		D2 PHE B 272	-25.973	74.767	-0.732		6
	MOTA		E1 PHE B 272	-23.200	74.606	-0.989		6
	MOTA		E2 PHE B 272	-25.321	73.518	-0.743		6
	MOTA		Z PHE B 272	-23.937	73.441	-0.856		6
	ATOM	91 C	PHE B 272	-28.144	78.472	-0.477		6
50		92 0		-28.803	78.393	0.558		8
20	MOTA	93 N		-28.027	79.621	-1.144		7
	ATOM		A THR B 273	-28.658	80.850	-0.652		6
	ATOM		B THR B 273	-28.023	82.105	-1.283		6
	ATOM		G1 THR B 273	-28.292	82.151	-2.688		8
55			G2 THR B 273	-26.511		-1.048		6
55	ATOM	98 0		-30.142		-0.971		6
	ATOM	99		-30.862		-0.535		8
	ATOM	100 N		-30.583			1.00 46.21	7
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5	ATOM	101	CA	LYS	В	274	-31.983	79.774	-2.147	1.00	54.53	6
	ATOM	102	СВ	LYS	В	274	-32.133	78.724	-3.232		54.36	6
	ATOM	103	С	LYS	В	274	-32.819	79.396	-0.931	1.00	56.88	6
	MOTA	104	0	LYS	В	274	-34.025	79.624	-0.906		57.98	8
	ATOM	105	N	ILE	В	275	-32.151	78.820	0.076	1.00	56.48	7
10	ATOM	106	CA	ILE	В	275	-32.791	78.381	1.332	1.00	52.64	6
	ATOM	107	CB	ILE	В	275	-32.638	76.863	1.519	1.00	49.15	6
	ATOM	108	CG2	ILE	В	275	-33.505	76.105	0.529	1.00	47.42	6
	MOTA	109	CG1	ILE	В	275	-31.188	76.441	1.343	1.00	45.31	6
	MOTA	110	CD1	ILE		275	-30.990	74.952	1.391	1.00	37.22	6
15	ATOM	111	С	ILE			-32.241	79.086	2.574	1.00	51.78	6
	ATOM	112	0	ILE		275	-32.858	79.049	3.622	1.00	49.80	8
	ATOM	113	N			276	-31.071	79.709	2.435	1.00	51.76	7
	ATOM	114	CA			276	-30.410	80.409	3.533	1.00	52.58	6
	ATOM	115	CB			276	-29.145	81.110	3.042	1.00	55.04	6
20	ATOM	116	CG2	ILE		276	-29.486	82.172	2.017	1.00	53.28	6
20	ATOM	117	CG1	ILE		276	-28.396	81.786	4.203		57.31	6
	ATOM	118	CD1	ILE		276	-27.862	80.854	5.231	1.00	60.32	6
	ATOM	119	C			276	-31.282	81.461	4.237		50.70	6
	ATOM	120	0			276	-31.015	81.817	5.385		55.55	8
25	ATOM	121	N	THR		277	-32.322	81.953	3.568		47.33	7
23	ATOM	122	CA	THR		277	-33.174	82.968	4.141		42.59	6
	MOTA	123	CB	THR		277	-34.042	83.632	3.048		44.97	6
	ATOM	124	OG1	THR		277	-33.202	84.145	2.001		46.38	8
	ATOM	125	CG2	THR		277	-34.856	84.781	3.653		37.17	6
30	MOTA	126	C	THR		277	-34.069	82.447	5.267		39.84	6
50	ATOM	127	Ö	THR		277	-34.083	83.026	6.375		40.55	8
	ATOM	128	N	PRO		278	-34.832	81.385	5.017		38.20	7
	ATOM	129	CD	PRO		278	-34.925	80.666	3.747		36.34	6
	ATOM	130	CA	PRO		278	-35.711	80.834	6.059		36.63	6
35	MOTA	131	CB	PRO		278	-36.475	79.715	5.357		32.95	6
35	MOTA	132	CG		В	278	-35.833	79.516	4.056		35.75	6
	ATOM	133	C		В	278	-34.892	80.324	7.220		38.60	6
	ATOM	134	Ö	PRO	В		-35.372	80.157	8.331		37.67	8
	ATOM	135	N	ALA			-33.636	80.040	6.927	1.00		7
40	ATOM	136	CA	ALA			-32.696	79.525	7.903		33.18	6
	ATOM	137	CB	ALA			-31.391	79.195	7.205		30.56	6
	ATOM	138	C	ALA			-32.447	80.536	8.991		33.47	6
	ATOM	139	Ö			279	-32.623	80.238	10.158		33.74	8
	ATOM	140	N			280	-32.010	81.728	8.577		29.96	7
45	ATOM	141	CA			280	-31.728	82.809	9.501		25.94	6
	ATOM	142	CB			280	-31.190	84.040	8.754		26.95	6
	ATOM	143	CG2			280	-30.881	85.149	9.715		15.40	6
	MOTA	144	CG1			280	-29.904	83.696	8.007		26.73	6
	ATOM	145	CD1			280	-29.255	84.878	7.362		34.31	6
50	ATOM	146	C			280	-32.964	83.172	10.310		31.39	6
50	ATOM	147	Ö			280	-32.882	83.378	11.522		35.69	8
	ATOM	148	И			281	-34.113	83.233	9.647		30.90	7
		149	CA			281	-34.113	83.586	10.328		33.49	6
	ATOM	150	CB			281	-36.598	83.396	9.419		37.18	6
55	ATOM	150	OG1			281	-36.703	82.034	9.005		.46.48	8
رر	ATOM	151	CG2			281	-36.703	84.289	8.198		32.85	6
	ATOM	152	CGZ			281	-35.523	82.706	11.556		29.94	6
	ATOM		0						12.634		25.55	8
	ATOM	154	U	ınĸ	Þ	281	-35.855	83.186	14.034	1.00	در. رے	0

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5	ATOM	155 N	I A	RG B 282		-35.296	81.405		1.00 32.70	7
•	MOTA			RG B 282		-35.439		12.475	1.00 34.27	6
	ATOM			RG B 282		-34.999		12.020	1.00 33.78	б
	MOTA			RG B 282		-35.986	77.944	12.280	1.00 45.15	6
	MOTA			RG B 282		-36.701	77.514	11.015	1.00 58.24	6
10	MOTA			RG B 282		-35.771	77.153	9.969	1.00 68.41	7
10	ATOM			RG B 282		-34.862	76.200	10.098	1.00 72.31	6
	MOTA			ARG B 282		-34.779	75.502	11.232	1.00 77.89	7
	ATOM			ARG B 282		-34.022	75.963	9.096	1.00 69.25	7
				ARG B 282		-34.556	80.919	13.622	1.00 34.81	6
1.5	ATOM			ARG B 282		-35.008	81.034	14.753	1.00 36.03	8
15	ATOM			/AL B 283		-33.288	81.183	13.289	1.00 31.71	7
	ATOM			/AL B 283		-32.304	81.667	14.249	1.00 30.16	6
	MOTA			VAL B 283		-30.993	82.029	13.559	1.00 29.00	6
	MOTA			VAL B 283		-30.015	82.617	14.557	1.00 28.64	6
20	MOTA			VAL B 283		-30.385	80.816	12.915	1.00 28.28	6
20	MOTA			VAL B 283		-32.848	82.884	14.994	1.00 32.50	6
	MOTA			VAL B 283		-32.619	83.057	16.185	1.00 33.48	8
	MOTA			VAL B 283		-33.573	83.728	14.265	1.00 30.96	7
	MOTA					-34.177	84.925	14.844	1.00 29.14	6
	MOTA	174		VAL B 284		-34.672	85.892	13.751	1.00 31.27	6
25	ATOM	175	_	VAL B 284		-35.278	87.129	14.371	1.00 24.21	6
	MOTA	176		VAL B 284		-33.554	86.270	12.812	1.00 30.51	6
	MOTA	177		VAL B 284		-35.336	84.498	15.747	1.00 28.89	6
	MOTA	178		VAL B 284		-35.330	84.994	16.860	1.00 27.29	8
	MOTA	179		VAL B 284		-36.143	83.564	15.250	1.00 28.76	7
30	MOTA	180		ASP B 285		-37.299	83.057	15.983	1.00 35.32	6
	MOTA	181		ASP B 285		-38.129	82.098	15.111	1.00 33.29	6
	MOTA	182		ASP B 285		-38.129	82.795	14.013	1.00 38.15	6
	ATOM	183	CG	ASP B 285		-39.660	83.729	14.305	1.00 34.70	8
	MOTA	184	OD1			-38.741	82.406	12.821	1.00 34.43	8
35	MOTA	185		ASP B 285		-36.863	82.339	17.257	1.00 36.70	6
	MOTA	186	С	ASP B 285		-37.606	82.304	18.237	1.00 37.96	8
	MOTA	187	0	ASP B 285			81.755	17.235	1.00 35.96	7
	MOTA	188	N	PHE B 286		-35.663	81.053	18.401	1.00 37.10	6
	MOTA	189	CA	PHE B 286		-35.134 -33.870	80.262	18.052	1.00 37.97	6
40	MOTA	190	CB	PHE B 28				19.258	1.00 36.50	6
	MOTA	191	CG	PHE B 28		-33.079 -33.704		20.294	1.00 36.75	6
	MOTA	192		PHE B 28		-33.704		19.343		6
	MOTA	193		PHE B 28		-31.721		21.401		6
	MOTA	194		PHE B 28				20.456		6
45		195		PHE B 28		-30.997		21.486		6
	MOTA	196	CZ	PHE B 28		-31.632				6
	MOTA	197	С	PHE B 28		-34.808				8
	MOTA	198	0	PHE B 28		-35.246				7
	MOTA	199	N	ALA B 28		-34.005				6
50	MOTA	200	CA	ALA B 28		-33.599				6
	MOTA	201	CB	ALA B 28		-32.644				6
	MOTA	202	С	ALA B 28		-34.831				8
	ATOM	203	0	ALA B 28		-34.882				7
	MOTA	204	N	LYS B 28		-35.820				6 -
55	MOTA	205	CA	LYS B 28		-37.066				6
	MOTA	206	CB	LYS B 28		-37.983				6
	MOTA	207	CG	LYS B 28		-37.57				6
	MOTA	208	CD	LYS B 28	8 8	-38.80	87.359	17.226	1.00 60.23	Ü

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5	ATOM	209	CE	LYS :	В	288	-39.680	86.308	16.564	1.00 6	2.81	6
	ATOM	210	NZ	LYS	В	288	-38.897	85.460	15.614	1.00 6	4.69	7
	ATOM	211	С	LYS	В	288	-37.846	84.901	21.191	1.00 4	3.31	6
	ATOM	212				288	-38.650	85.532	21.857	1.00 4	5.66	8
	ATOM	213				289	-37.618	83.604	21.345	1.00 4		7
10	ATOM	214				289	-38.313	82.849	22.351	1.00 4		6
10		214				289	-38.554	81.418	21.845	1.00 4		6
	ATOM						-39.438	81.368	20.589	1.00 3		6
	ATOM	216	CG	LYS					20.309	1.00 4		6
	ATOM	217	CD	LYS			-40.093	80.010				
	MOTA	218	CE	LYS		289	-41.025	79.987	19.223	1.00 4		6
15	ATOM	219	NZ	LYS		289	-42.391	80.476	19.512	1.00 5		7
	MOTA	220	С	LYS		289	-37.555	82.871	23.668	1.00 4		6
	MOTA	221	0			289	-38.057	82.366	24.657	1.00 3		8
	MOTA	222	N	LEU		290	-36.365	83.482	23.661	1.00 4		7
	ATOM	223	CA	LEU		290	-35.539	83.599	24.854	1.00 3		6
20	MOTA	224	CB	LEU	В	290	-34.053	83.499	24.491	1.00 3		6
	ATOM	225	CG	LEU	В	290	-33.640	82.240	23.767		84.81	6
	MOTA	226	CD1	LEU	В	290	-32.147	82.255	23.523	1.00 2		6
	ATOM	227	CD2	LEU	В	290	-34.013	81.040	24.607	1.00 3	33.45	6
	MOTA	228	С	LEU	В	290	-35.832	84.915	25.577	1.00 4	10.08	6
25	MOTA	229	0	LEU	В	290	-35.479	86.006	25.088	1.00 4	12.00	8
	ATOM	230	N	PRO	В	291	-36.462	84.840	26.765	1.00 4	10.27	7
	MOTA	231	CD	PRO	В	291	-36.819	83.613	27.494	1.00 3	39.65	6
	MOTA	232	CA	PRO	В	291	-36.782	86.069	27.501	1.00 3	38.28	6
	MOTA	233	CB	PRO	В	291	-37.376	85.574	28.811	1.00 3	35.88	6
30	ATOM	234	CG	PRO	В	291	-37.549	84.110	28.695	- 1.00 3	34.19	6
	MOTA	235	С	PRO	В	291	-35.570	87.002	27.714	1.00 4	10.05	6
	MOTA	236	0	PRO	В	291	-35.625	88.197	27.403	1.00 4	11.33	8
	MOTA	237	N	MET	В	292	-34.474	86.476	28.258	1.00 4	10.59	7
	MOTA	238	CA	MET	В	292	-33.296	87.286	28.545	1.00 4	12.86	6.
35	MOTA	239	СВ	MET	В	292	-32.149	86.376	28.975	1.00	13.28	6
	MOTA	240	CG	MET	В	292	-32.553	85.302	29.970	1.00 5	50.35	6
	MOTA	241	SD	MET	В	292	-31.070	84.609	30.755	1.00	51.17	16
	ATOM	242	CE	MET	В	292	-31.797	83.212	31.701	1.00 9	54.63	6
	ATOM	243	С	MET	В	292	-32.895	88.077	27.315	1.00	41.05	6
40	MOTA	244	0	MET	В	292	-32.228	89.098	27.420	1.00	39.66	8
	MOTA	245	N	PHE	В	293	-33.322	87.604	26.143	1.00	39.30	7
	ATOM	246	CA	PHE	В	293	-33.017	88.271	24.878	1.00	40.92	6
	MOTA	247	CB	PHE	В	293	-33.296	87.329	23.707	1.00	40.98	6
	MOTA	248	CG	PHE	В	293	-32.937	87.909	22.365	1.00	42.78	6
45	ATOM	249	CD1	PHE	В	293	-31.653	88.354	22.120	1.00	44.40	6
	ATOM	250	CD2	PHE	В	293	-33.872	87.972	21.350	1.00	43.66	6
	ATOM	251	CE1	PHE	В	293	-31.306	88.869	20.872	1.00	39.83	6
	MOTA	252	CE2	PHE	В	293	-33.525	88.486	20.100	1.00	46.21	6
	MOTA	253	CZ			293	-32.239	88.926	19.859	1.00	45.18	6
50	ATOM	254	С	PHE	В	293	-33.873	89.518	24.744	1.00	45.54	6
-	ATOM	255	0			293	-33.369	90.626		1.00	42.01	8
	ATOM	256	N			294	-35.181	89.305		1.00		7
	ATOM	257	CA			294	-36.146	90.382		1.00		6
	MOTA	258	CB			294	-37.553	89.793		1.00		6
55	ATOM	259	SG			294	-37.899	88.607		1.00		16
	ATOM	260	C			294	-35.974	91.474	25.751	1.00		6
	MOTA	261	0			294	-36.585	92.536		1.00		8
	MOTA	262	N			295	-35.137	91.200		1.00		7
	AIOM	202	7.4	0110	ט	د د ه	33.137	21.200	20.700	2.00	· · -	•

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5	ATOM	263 CA	GLU B 295	-34.839			- - - -	6
,	MOTA	264 CB	GLU B 295	-34.553	J		1.00 57.40	6
	ATOM	265 CG	GLU B 295	-35.811			1.00 69.63	6
	ATOM	266 CD	GLU B 295	-36.610	92.144	_	1.00 78.49	6
	MOTA	267 OE		-36.153	92.869		1.00 82.82	8
10	MOTA	268 OE2		-37.730	92.385		1.00 85.30	8
10	ATOM	269 C	GLU B 295	-33.629	93.009	27.415	1.00 48.54	6
	ATOM	270 0	GLU B 295	-32.981	93.627	28.260	1.00 49.82	8
	MOTA	271 N	LEU B 296	-33.374	93.030	26.109	1.00 43.79	7
	MOTA	272 CA	LEU B 296	-32.268	93.761	25.540	1.00 45.42	6
15	MOTA	273 CB	LEU B 296	-31.319	92.769	24.838	1.00 41.04	6
13	MOTA	274 CG		-30.735	91.631	25.662	1.00 42.74	6
	ATOM		1 LEU B 296	-30.354	90.478	24.764	1.00 40.99	6
	ATOM		2 LEU B 296	-29.559	92.119	26.468	1.00 39.44	6
	MOTA	277 C	LEU B 296	-32.760	94.779	24.522	1.00 45.56	6
20	ATOM	278 0	LEU B 296	-33.845	94.600	23.924	1.00 43.07	8
20	MOTA	279 N	PRO B 297	-32.004	95.875	24.338	1.00 46.99	7
		280 CI		-30.740	96.123	25.046	1.00 47.12	6
	ATOM ATOM	281 CF		-32.388	96.912	23.363	1.00 49.61	6
		282 CE		-31.294	97.973	23.494	1.00 49.91	6
25	MOTA	283 C	_	-30.302	97.477	24.545	1.00 51.28	6
25	MOTA MOTA	284 C	PRO B 297	-32.263	96.273	21.913	1.00 49.59	6
		285 0	PRO B 297	-31.441	95.340	21.685	1.00 51.66	8
	ATOM ATOM	286 N	CYS B 298	-33.035	96.667	20.854	1.00 51.02	7
	MOTA	287 C		-32.761	96.150	19.456	1.00 52.86	6
20	MOTA	288 C		-33.140	97.165	18.356	1.00 54.57	6
30	ATOM	289 S		-34.884	97.085	17.836	1.00 67.87	16
	MOTA	290 C		-31.385	96.330	19.127	1.00 48.51	6
	MOTA	291 0		-30.579	95.506		1.00 49.58	8
	MOTA	292 N		-31.107			1.00 44.17	7
35	MOTA		A GLU B 299	-29.989	97.645		1.00 47.57	6
33	ATOM		B GLU B 299	-29.402	98.973		1.00 49.92	6
	MOTA		G GLU B 299	-29.944			1.00 59.30	6
	MOTA		D GLU B 299	-31.090			1.00 63.80	6
	ATOM		E1 GLU B 299	-31.673			1.00 69.03	8 8
40			E2 GLU B 299		3 100.458		1.00 67.10	-
40	ATOM		GLU B 299	-28.993				6
	MOTA		GLU B 299	-28.200		_		8 7
	MOTA		N ASP B 300	-29.04				6
	MOTA		CA ASP B 300	-28.15				6
45			CB ASP B 300	-27.98				6
,,	ATOM		CG ASP B 300	-27.23				8
	MOTA		OD1 ASP B 300	-26.20				8
	MOTA		OD2 ASP B 300	-27.66				6
	ATOM		C ASP B 300	-28.72				8
5(O ASP B 300	-28.00				7
٥,	ATOM		N GLN B 301	-30.01				
	ATOM	_	CA GLN B 301	-30.71				6
	MOTA	311	CB GLN B 301	-32.23				6
	ATOM	312	CG GLN B 301	-32.90				
5:			CD GLN B 301	-34.40				
٠.	MOTA C		OE1 GLN B 301	-34.85				
	ATOM		NE2 GLN B 301	-35.16				
	MOTA		C GLN B 301	-30.23	37 91.83	18.45	5 1.00 41.64	Ø
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5	ATOM	317	0	GLN E		-30.162	90.662	18.100	1.00	45.02	8 =
	MOTA	318	N	ILE E	302	-29.916	92.864	17.674	1.00	41.01	7
	ATOM	319	CA	ILE E	302	-29.424	92.692	16.311	1.00	40.23	6
	MOTA	320	CB	ILE E	302	-29.584	93.978	15.498	1.00	39.52	6
	MOTA	321	CG2	ILE E	302	-29.034	93.792	14.100	1.00	31.98	6
10	MOTA	322	CG1	ILE E		-31.059	94.385	15.416	1.00	40.77	6
	ATOM	323	CD1	ILE E		-31.939	93.317	14.775	1.00	45.43	6
	ATOM	324	С	ILE E		-27.966	92.260	16.342	1.00	38.58	6
	ATOM	325	0	ILE E		-27.613	91.197	15.830	1.00	40.81	
	ATOM	326	N	ILE E		-27.128	93.111	16.933	1.00	37.50	8 7
15	ATOM	327	CA	ILE E		-25.692	92.846	17.062			
	ATOM	328	CB	ILE E		-25.066	93.648	18.203	1.00	39.33	6
	ATOM	329	CG2	ILE I		-23.566	93.405		1.00	39.06	6
	ATOM	330	CG1	ILE I				18.257	1.00	36.19	6
	ATOM	331	CD1	ILE		-25.309	95.143	18.020	1.00	40.15	6
20	ATOM	332				-24.816	95.966	19.173	1.00	36.93	6
20			С	ILE I		-25.470	91.365	17.323	1.00	36.49	6
	MOTA	333	0	ILE I		-24.619	90.725	16.712	1.00	36.58	8
	ATOM	334	N	LEU I		-26.244	90.843	18.266	1.00	32.91	7
	ATOM	335	CA	LEU I		-26.194	89.433	18.633	1.00	27.55	6
25	ATOM	336	CB	LEU I		-27.172	89.182	19.793	1.00	22.35	6
25	ATOM	337	CG	LEU I		-26.623	89.449	21.187	1.00	26.88	6
	ATOM	338	CD1	LEU I		-25.540	90.495	21.136	1.00	24.82	6
	ATOM	339	CD2	LEU 1		-27.747	89.840	22.121	1.00	23.69	6
	MOTA	340	С	LEU I		-26.505	88.547	17.425	1.00	28.05	6
	MOTA	341	0	LEU 1		-25.668	87.751	16.983	1.00	24.68	8
30	ATOM	342	N	LEU I			88.700	16.897	1.00	26.34	7
	MOTA	343	CA	LEU 1			87.939	15.741	1.00	30.91	6
	ATOM	344	CB	LEU I			88.514	15.199	1.00	32.50	6
	ATOM	345	CG	LEU 1		-30.699	88.305	16.050	1.00	33.36	6
2.5	ATOM	346	CD1	LEU 1			88.839	15.342	1.00	33.87	6
35	ATOM	347	CD2	LEU 1			86.812	16.298	1.00	31.72	6
	ATOM	348	С	LEU 1			87.922	14.666	1.00	29.76	6
	ATOM	349	0	LEU 1			86.860	14.202	1.00	29.33	8
	ATOM	350	N	LYS I			89.107	14.291	1.00	29.72	7
40	MOTA	351	CA		306		89.254	13.264	1.00	34.28	6
40	MOTA	352	CB		306		90.732	13.077	1.00	35.98	6
	MOTA	353	CG		306		91.581	12.494	1.00	43.35	6
	ATOM	354	CD	LYS I			92.987	12.182	1.00	51.50	6
	MOTA	355	CE		306	· -	92.932	11.190	1.00	53.26	6
	ATOM	356	ΝZ	LYS I			94.161	11.251	1.00	59.61	7
45	ATOM	357	С	LYS I	3 306	-24.308	88.484	13.556	1.00	35.25	6
	ATOM	358	0	LYS I	306	-23.681	87.917	12.653	1.00	33.95	8
	MOTA	359	N	GLY 1	3 307	-23.918	88.478	14.829		35.79	7
•	MOTA	360	CA	GLY I	307	-22.702	87.793	15.227		34.59	6
	MOTA	361	С	GLY I	3 307	-22.811	86.291	15.383		33.80	6
50	MOTA	362	0	GLY I	3 307	-21.944	85.564	14.895		31.59	8
	ATOM	363	N	CYS I	3 3 3 8	-23.861	85.843	16.071		31.15	7
	ATOM	364	CA	CYS I	3 3 3 8	-24.069	84.434	16.320		29.04	6
	ATOM	365	CB	CYS I		-24.761	84.240	17.663		27.59	6
	ATOM	366	SG	CYS I		-26.496	84.629	17.608		30.50	16
55	ATOM	367	C		3 308	-24.911	83.712	15.266		30.59	6
	ATOM	368	Ö		3 308	-25.088	82.499	15.365		33.77	
	ATOM	369	N		3 309	-25.432	84.429	14.266		28.46	8 7
	ATOM	370	CA		3 309	-26.270	83.787	13.265		30.10	6
		•	•	1		20.270	55.767	19.203	1.00	50.10	0
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5	ATOM	371	CB	CYS			-26.706	84.761	12.194		33.43	6
	ATOM	372	SG	CYS			-27.875	84.011	11.089		35.20	16
	ATOM	373	С	CYS			-25.617	82.608	12.603		27.72	6
	MOTA	374	0	CYS		309	-26.170	81.518	12.610	1.00		8
10	MOTA	375	N			310	-24.447	82.829	12.011	1.00	26.15	7
10	MOTA	376	CA	MET	В	310	-23.737	81.748	11.352	1.00	26.06	6
	ATOM	377	CB	MET	В	310	-22.439	82.263	10.712	1.00	25.32	6
	MOTA	378	CG	MET	В	310	-21.584	81.157	10.080	1.00	24.08	6
	MOTA	379	SD	MET	В	310	-22.555	80.324	8.758	1.00	27.71	16
	MOTA	380	CE		В	310	-21.549	78.826	8.427	1.00	28.50	6
15	MOTA	381	С		В	310	-23.416	80.673	12.374	1.00	25.94	6
	MOTA	382	0	MET		310	-23.659	79.489	12.151	1.00	28.09	8
	MOTA	383	N	GLU		311	-22.865	81.117	13.500	1.00	25.39	7
	MOTA	384	CA	GLU	В	311	-22.466	80.231	14.576	1.00	27.03	6
	MOTA	385	CB	GLU	В	311	-22.036	81.048	15.797	1.00	24.39	6
20	MOTA	386	CG	GLU		311	-21.019	82.141	15.509	1.00	26.00	6
	ATOM	387	.CD	GLU		311	-20.524	82.835	16.740	1.00	23.95	6
	MOTA	388	OE1	GLU		311	-21.321	83.108	17.668	1.00	19.72	8
	MOTA	389	OE2	GLU		311	-19.313	83.163	16.815	1.00	26.51	8
	MOTA	390	С	${ t GLU}$		311	-23.582	79.264	14.964	1.00	27.51	6
25	MOTA	391	0	GLU		311	-23.347	78.068	15.093	1.00	29.67	8
	MOTA	392	N	ILE		312	-24.794	79.792	15.145	1.00	26.82	7
	MOTA	393	CA	ILE		312	-25.933	78.967	15.527	1.00	25.71	6
	MOTA	394	СВ	ILE	В	312	-27.125	79.814	16.021	1.00	23.35	6
	MOTA	395	CG2	ILE		312	-28.327	78.933	16.276	1.00	20.27	6
30	MOTA	396	CG1	ILE		312	-26.771	80.541	17.325	1.00	20.88	6
	MOTA	397	CD1			312	-27.952	81.163	18.028	1.00	18.15	6
	MOTA	398	С	ILE		312	-26.370	78.072	14.392	1.00	27.91	6
	ATOM	399	0	ILE	В	312	-26.769	76.926	14.605	1.00	28.96	8
25	ATOM	400	N	MET	В	313	-26.303	78.603	13.174	1.00	27.66	7
35	MOTA	401	CA	MET		313	-26.696	77.832	11.999	1.00	30.18	6
	MOTA	402	CB		В	313	-26.696	78.691	10.734		36.89	6
	ATOM	403	CG	MET		313	-27.882	79.634	10.607	1.00	37.95	6
	ATOM	404	SD		В	313	-28.238	80.275	8.907	1.00	42.38	16
40	ATOM ATOM	405 406	CE C	MET	В	313	-26.787	81.316	8.639	1.00	40.68	6
40	ATOM	407		MET MET	В	313	-25.791	76.632	11.808		27.43	6
	ATOM	407	O N			314	-26.258	75.501	11.893		28.61	8
	ATOM	409	CA			314	-24.508	76.882	11.549		24.88	7
	ATOM	410	CB			314	-23.533	75.824	11.346		27.98	6
45	ATOM	411	OG			314	-22.150 -21.844	76.441	11.165		29.64	6
1.5	ATOM	412	C			314	-21.644 -23.514	77.316	12.227		43.44	8
	ATOM	413	0	SER			-23.279	74.774	12.465		22.30	6
	ATOM	414	N	LEU			-23.760	73.592	12.199		24.18	8
	ATOM	415	CA	LEU			-23.792	75.187 74.219	13.714		23.99	7
50	ATOM	416	CB	LEU			-24.095		14.811		25.07	6
50	ATOM	417	CG	LEU			-24.507	74.869 73.860	16.169		19.11	6
	ATOM	418		LEU			-23.390		17.234		20.39	6
	ATOM	419		LEU				72.878	17.493		18.92	6
	ATOM	420	CDZ	LEU			-24.895 -24.892	74.560	18.514		12.93	6
55	ATOM	421	0	LEU			-24.892 -24.672	73.219	14.517		24.53	6
	ATOM	422	N			316	-24.672 -26.079	72.014	14.550		26.32	8
	ATOM	423	CA	ARG			-26.079	73.762	14.254		28.18	7
	ATOM	424	CB			316	-27.278	72.996 73.941	13.971		27.54	6
		767	OD.	טוזה	ט	210	104	13.541	13.651	1.00	27.39	6
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_		425 CG ARG B 316	-28.823 74.857 14.809 1.00 22.00 6
5	MOTA	216	-30.074 75.657 14.451 1.00 18.76
	MOTA	420 05 1110	-30.905 75.944 15.598 1.00 26.57
	MOTA	427 100 216	-32.166 76.337 15.489 1.00 30.81 6
	MOTA	420 02	-32.686 76.535 14.280 1.00 33.71
	ATOM	- 016	-32.900 76.542 16.581 1.00 33.13
10	MOTA	400 11111 1-1-	27 128 72 028 12.830 1.00 28.09
	MOTA	401	27 852 71 053 12.760 1.00 32.41 8
	MOTA	432 O ARG B 316	26 187 72 309 11.941 1.00 28.36
	MOTA	433 N ALA B 317	25 938 71 466 10.794 1.00 26.64 6
	MOTA	434 CA ALA B 317	25 237 72 300 9.675 1.00 22.93 6
15	MOTA	435 CB ALA B 317	24 009 70 327 11.150 1.00 28.35 6
	MOTA	436 C ALA B 317	25 223 69 187 10.773 1.00 32.10 8
	MOTA	437 O ALA B 317	7 11 222 1 20 29 12
	MOTA	438 N ALA B 318	-23.941 70.000 1 00 27 50 6
	MOTA	439 CA ALA B 318	-22.957 05.002 1.00 29 39 6
20	MOTA	440 CB ALA B 318	-21.915 70.555 13.004 1.00 28 10 6
20	ATOM	441 C ALA B 318	-23.645 60.651 100.28 18 8
	ATOM	442 O ALA B 318	-23.413 07.413 1.00 20 16 7
	MOTA	443 N VAL B 319	-24.502 05.012 1.00 35 24 6
	MOTA	444 CA VAL B 319	-25.259 00.107 1 00 27 34 6
25	ATOM	445 CB VAL B 319	-26.228 68.897 13.703 1.00 20 96 6
23	ATOM	446 CG1 VAL B 319	-25.570 70.113
	MOTA	447 CG2 VAL B 319	-27.505 69.212 13.022 1.00 40 01 6
	MOTA	448 C VAL B 319	-26.066 67.140 14.550 1.00 42 70 8
	ATOM	449 O VAL B 319	-26.701 66.230 14.370 1 00 39 64 7
30		450 N ARG B 320	-26.025 67.353 12.725 1.00 39 61 6
30	MOTA	451 CA ARG B 320	-26.770 66.541 11.702 1.00 37 26 6
	ATOM	452 CB ARG B 320	-27.838 67.409 11.123 1.00 43 12 6
	ATOM	453 CG ARG B 320	-29.152 67.280 11.022 1.00 50 79 6
	ATOM	454 CD ARG B 320	-30.145 68.340 11.307 1.00 54 71 7
35		455 NE ARG B 320	-31.500 67.911 11.703 1.00 57.99 6
32	ATOM	456 CZ ARG B 320	-32.555 68.723 11.337 1.00 49 08 7
	MOTA	457 NH1 ARG B 320	-32.398 69.957 11.130 1.00 50 50 7
	MOTA	458 NH2 ARG B 320	-33.773 68.302 11.044 1.00 62.14 6
	ATOM	459 C ARG B 320	-25.937 65.910 10.670 1.00 46.30 8
4		460 O ARG B 320	-26.381 65.802 9.532 1.00 13.00
41	MOTA U	myrp D 221	-24.734 65.488 11.022 1.00 42 70 6
	ATOM	on myn n 221	-23.858 64.848 10.003 1.00 38 01 6
	ATOM	an man n 321	-22.433 65.332 10.237 24 6
•	ATOM	myn n 201	-21.393 64.396 9.730 1.00 33.85 6
1		myn n 221	-21.265 64.176 5.337 1.00 34 49 6
4	ATOM ATOM	myn n 221	-20.333 63.256 7.512 1.00 28 03 6
	ATOM	myn n 221	-20.583 63.663 10.013 1.00 32 69 6
	ATOM	myn n 221	-19.658 62.769 10.134 1.00 35 18 6
		a- myn n 201	-19.532 62.551 8.761 1.00 39.48 8
	MOTA	an mun n 201	-18.616 61.661 8.292 1.00 35.11
;	50 ATON		-23.897 63.347 10.234 1.00 49.02
	ATON		-23.560 62.857 11.292 1.00 40.02
	ATO	" " " " " " " " " " " " " " " " " " "	-24.317 62.642 9.188 1.00 44.50
	ATOI	an nan n 322	-24.391 61.170 9.182 1.00 45.80
	ATO	on ach h 322	-25.570 60.749 8.294 1.00 46.64 6
	55 ATO		-25.449 59.359 7.775 1.00 40.00
	ATO	ont non p 301	-24.388 58.737 7.986 1.00 40.00
	OTA	and man n 22'	7 117 1.00 40.00
	ATO	M 478 OD2 ASP B 322	105

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5	MOTA	479	С	ASP				-23.044	60.659	8.682		45.82	6
	ATOM	480	0		В	322		-22.738	60.783	7.495		4,5.38	8
	ATOM	481	N	PRO		323		-22.242	60.005	9.549	1.00	46.53	7
	MOTA	482	CD	PRO	В	323		-22.594	59.676	10.934	1.00	47.16	6
	ATOM	483	CA	PRO	В	323		-20.910	59.487	9.162	1.00	46.63	6
10	MOTA	484	CB	PRO	В	323		-20.367	58.847	10.433	1.00	43.95	6
	ATOM	485	CG	PRO	В	323		-21.398	58.958	11.454	1.00	43.93	6
	ATOM	486	С	PRO	В	323		-20.933	58.489	8.017	1.00	48.34	6
	ATOM	487	0	PRO	В	323		-20.040	58.457	7.171	1.00	50.84	8
	ATOM	488	N	GLU		324		-21.951	57.631	8.022		52.39	7
15	ATOM	489	CA		В	324		-22.126	56.615	7.008	1.00	55.85	6
	ATOM	490	СВ	GLU		324		-23.491	55.960	7.216	1.00	55.54	6
	ATOM	491	CG	GLU	В	324		-23.678	55.332	8.581	1.00	40.00	6
	MOTA	492	CD	GLU	В	324		-22.642	54.294	8.888	1.00	40.00	6
	ATOM	493	OE1	GLU	В	324		-21.796	53.979	8.000	1.00		8
20	ATOM	494	OE2	GLU	В	324		-22.645	53.751	10.029	1.00	40.00	8
20	ATOM	495	C	GLU	В	324		-22.043	57.292				
	ATOM	496	0		В	324		-21.144		5.655	1.00		6
			-						57.149	4.896		59.81	8
	ATOM	497	N	SER		325		-23.165	58.022	5.389		52.95	7
25	ATOM	498	CA	SER		325		-23.358	58.762	4.163		50.10	6
25	MOTA	499	CB	SER		325		-24.768	59.357	4.163	1.00		6
	MOTA	500	OG	SER		325		-25.051	59.976	5.403			8
	ATOM	501	С	SER				-22.324	59.861	3.964	1.00	50.61	6
	MOTA	502	0	SER		325		-21.956	60.176	2.848	1.00	52.19	8
2.0	MOTA	503	N	GLU		326		-21.851	60.422	5.070	1.00	45.64	7
30	ATOM	504	CA	GLU	В	326		-20.854	61.476	5.050			6
	ATOM	505	CB	GLU	В	326	•	-19.602	61.022	4.277	1.00	42.74	6
	ATOM	506	CG	GLU	В	326		-18.880	59.814	4.876	1.00	50.32	6
	ATOM	507	CD	GLU	В	326		-17.576	59.524	4.207	1.00	56.34	6
	ATOM	508	OE1		В	326		-16.898	58.545	4.608	1.00	59.31	8
35	MOTA	509	OE2	GLU	В	326		-17.177	60.255	3.266	1.00	55.74	8
	MOTA	510	С	GLU	В	326		-21.401	62.731	4.418	1.00	40.23	6
	MOTA	511	0	GLU	В	326		-20.793	63.285	3.514	1.00	40.44	8
	MOTA	512	N	THR	В	327		-22.528	63.208	4.934	1.00	35.90	7
	ATOM	513	CA	THR	В	327		-23.163	64.418	4.401	1.00	37.29	6
40	MOTA	514	CB	THR	В	327		-24.146	64.052	3.285	1.00	37.63	6
	ATOM	515	OG1	THR	В	327		-25.172	63.199	3.803	1.00	38.12	8
	ATOM	516	CG2	THR	В	327		-23.445	63.342	2.130	1.00	39.90	6
	MOTA	517	С	THR	В	327		-23.961	65.125	5.473	1.00	39.49	6
	MOTA	518	0	THR	В	327		-24.645	64.473	6.264	1.00	40.50	8
45	ATOM	519	N	LEU	В	328		-23.909	66.454	5.473	1.00	36.64	? 6
	MOTA	520	CA	LEU	В	328		-24.675	67.239	6.447	1.00	37.73	6
	MOTA	521	CB	LEU	В	328		-24.061	68.637	6.620	1.00	37.78	6
	MOTA	522	CG	LEU	В	328		-22.586	68.750	6.931		36.26	6
	ATOM	523	CD1	LEU	В	328		-22.260	70.145	7.411		36.56	6
50	ATOM	524	CD2	LEU				-22.231	67.751	8.000		39.85	6
	ATOM	525	С			328		-26.090	67.344	5.897		37.27	6
	ATOM	526	0			328		-26.358	66.855	4.805		34.96	8
	ATOM	527	N			329		-26.989	67.975	6.647		39.73	7
	ATOM	528	CA			329		-28.369	68.132	6.215		40.81	6
55	ATOM	529	CB			329		-29.279	67.135	6.918		42.67	6
	ATOM	530	0G1			329		-28.799	65.809	6.686		42.52	8
	MOTA	531	CG2			329		-30.702	67.255	6.375		43.52	6
	ATOM	532	C			329		-28.853	69.529	6.498		43.32	6
	111 011	JJ2	_	1111	יי	263			09.029	0.470	1.00	44.01	0
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		n 220	-29.432 69.801 7.535 1.00 43.72 8
5	MOTA	533 O THR B 329	-28 589 70.413 5.546 1.00 44.62
	MOTA	534 N LEU B 330 535 CA LEU B 330	-28 983 71.812 5.658 1.00 45.09 6
	ATOM	333 011 == 220	20 254 72 608 4.510 1.00 44.66 6
	MOTA	536 CB LEU B 330	26.047 72 735 4.539 1.00 51.06 6
	ATOM	537 CG LEU B 330	26 226 71 367 4.640 1.00 48.58 6
10	MOTA	538 CD1 LEU B 330	3.299 1.00 45.18 6
	MOTA	539 CD2 LEU B 330	20.508 71 965 5.652 1.00 48.06 6
	MOTA	540 C LEU B 330	30.308 71.308 4.959 1.00 49.33 8
	MOTA	541 O LEU B 330	7 1 21
	MOTA	542 N ASN B 331	-30.986 /2.511
15	MOTA	543 CA ASN B 331	-32.407 73.211
13	MOTA	544 CB ASN B 331	-32.870 74.010 5 740 1 00 60 35 6
	ATOM	545 CG ASN B 331	-33.667 73.223 6 430 1 00 61 84 8
	MOTA	546 OD1 ASN B 331	-33.182 70.133 - 304 1 00 65 92 7
	MOTA	547 ND2 ASN B 331	-34.935 /3.232 1 00 50 00 6
20	MOTA	548 C ASN B 331	-33.251 /1.353 6 570 1 00 60 17 8
20	MOTA	549 O ASN B 331	-34.484 /2:000 7 054 1 00 58 45 7
	ATOM	550 N GLY B 332	-32.596 70.040 - 205 1 00 59 55 6
	MOTA	551 CA GLY B 332	-33.295 09.307
	ATOM	552 C GLY B 332	-33.909 09.001 1 00 61 32 8
25	ATOM	553 O GLY B 332	-34.609 60.000 1 00 60 28 7
23	ATOM	554 N GLU B 333	-33.639 09.020 1 1 00 50 13 6
	MOTA	555 CA GLU B 333	-34.196 05.102 1 00 62 40 6
	MOTA	556 CB GLU B 333	-34.900 70.320 - 600 7 00 75 69 6
	ATOM	557 CG GLU B 333	-36.099 70.303 1 00 80 41 6
30		558 CD GLU B 333	-36.720 72.133 - 1.00 79 98 8
30	ATOM	559 OE1 GLU B 333	-33.904 /3.001 00 83 81 8
	MOTA	560 OE2 GLU B 333	-37.900 72.100 - 100 57 18 6
	MOTA	561 C GLU B 333	-33.110 00.722
	MOTA	562 O GLU B 333	-33.230 07.003 - 500 1 00 55 20 7
3:		563 N MET B 334	-32.034 03.320 - 1 00 50 85 6
٦.	MOTA	564 CA MET B 334	-30.926 03.23
	ATOM	565 CB MET B 334	-30.514 70.505 0 104 1 00 45 39 6
	MOTA	566 CG MET B 334	-29.244 70.400 0.201 1 00 44 56 16
	MOTA	567 SD MET B 334	-28.743 72.000 0.02
Δ	O ATOM	568 CE MET B 334	-30.307 72.410 2.310 1.00 51 59 6
•	ATOM	569 C MET B 334	-29.711 00.001 1 00 52 52 8
	ATOM	570 O MET B 334	-29.103 03.101 1 7 7 7 1 00 51 00 7
	MOTA	571 N ALA B 335	-29.270 67.313 2.267 1.00 48.98 6
	ATOM	572 CA ALA B 335	28.106 60.302 2.274 1.00 47.86 6
4	45 ATOM	573 CB ALA B 335	26.377 63.301 1.371 1.00 51.01 6
	ATOM	574 C ALA B 335	26.936 66.760 0.190 1.00 51.61 8
	ATOM	7 575 O ALA B 335	25 227 67 770 1 930 1.00 46.62 7
	ATOM	1 576 N VAL B 336	-23.921 07.773 1 100 42 35 6
	MOTA	1 577 CA VAL B 336	24.750 00.235 1 258 1.00 42.41 6
	50 ATON	4 578 CB VAL B 336	-24.466 05.033 2.00 1 00 42.00 6
	ATO	vr 579 CG1 VAL B 336	25.095 70.110 2.642 1.00 40.32 6
	ATO	$_{ m M}$ 580 CG2 VAL B 336	-24.018 70.001 1 611 1.00 45.33 6
	ATO	M 581 C VAL B 336	2 5.495 67.336 2 681 1.00 47.42 8
	ATO	M 582 O VAL B 336	-23.464 66.775 2.001 2.00 41.60 7
	55 ATO	M 583 N THR B 337	-22.401 07.110 1 00 39.69 6
	ATO	M 584 CA THR B 337	-21.172 00.010 -0 173 1.00 41.35 6
	ATO	M 585 CB THR B 337	7 -20.720 66.022 -1 213 1.00 49.35 8
	ATC	001 WID D 33.	7 -20.273 33133
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5	ATOM	587	CG2 T	HR B 337	-21.869	65.175	-0.702	1.00 40.38	6
,	ATOM	588		HR B 337	-20.087	67.846	1.318	1.00 37.88	6
	MOTA	589		HR B 337	-20.141	68.975	0.832	1.00 34.06	8
	MOTA	590		RG B 338	-19.097	67.417	2.095	1.00 37.61	7
		591		RG B 338	-17.942	68.241	2.442	1.00 38.68	6
10	ATOM	592		RG B 338	-16.770	67.333	2.823	1.00 35.95	6
10	ATOM			RG B 338	-15.455	68.042	3.064	1.00 38.83	6
	MOTA	593		RG B 338	-14.348	67.029	3.319	1.00 35.88	6
	MOTA	594			-14.520	66.239	4.530	1.00 37.42	7
	MOTA	595		RG B 338	-14.274	66.669	5.766	1.00 30.20	6
_	MOTA	596		ARG B 338	-13.794	67.892	5.973	1.00 27.98	7
15	MOTA	597	NH1 F			65.847	6.788	1.00 27.40	7
	MOTA	598	NH2 F		-14.481		1.229	1.00 38.09	6
	ATOM	599		ARG B 338	-17.581	69.075		1.00 34.12	8
	MOTA	600		ARG B 338	-17.537	70.299	1.284	1.00 34.12	7
	ATOM	601		GLY B 339	-17.345	68.383	0.117		6
20	MOTA	602	CA (GLY B 339	-16.981	69.054	-1.119	1.00 41.35	
	MOTA	603	C (GLY B 339	-18.004	70.109	-1.460	1.00 41.23	6
	MOTA	604	0	GLY B 339	-17.736	71.291	-1.330	1.00 38.30	8
	ATOM	605	N	GLN B 340	-19.174	69.665	-1.909	1.00 38.58	7
	ATOM	606	CA	GLN B 340	-20.258	70.564	-2.276	1.00 40.79	6
25	MOTA	607	СВ	GLN B 340	-21.596	69.843	-2.079	1.00 40.82	6
23	ATOM	608		GLN B 340	-21.830	68.657	-3.029	1.00 41.10	6
	ATOM	609		GLN B 340	-23.154	67.937	-2.783	1.00 48.84	6
	ATOM	610		GLN B 340	-23.353	67.313	-1.715	1.00 50.53	8
	ATOM	611		GLN B 340	-24.050	68.015	-3.753	1.00 54.25	7
30	ATOM	612	C	GLN B 340	-20.239	71.872	-1.475	1.00 41.50	6
30		613	0	GLN B 340	-20.114	72.958	-2.032	1.00 42.72	8
	MOTA	614	Ŋ	LEU B 341	-20.352	71.736	-0.156	1.00 42.00	7
	ATOM		CA	LEU B 341	-20.375	72.879	0.746	1.00 38.10	6
	MOTA	615		LEU B 341	-20.401	72.419	2.201	1.00 36.66	6
2.5	ATOM	616	CB	LEU B 341	-20.678	73.514	3.194	1.00 39.94	6
35	ATOM	617	CG		-22.088	74.038	2.936	1.00 34.98	6
	MOTA	618			-20.570		4.609	1.00 40.95	6
	MOTA	619			-19.170		0.543	1.00 36.37	6
	MOTA	620	С	LEU B 341	-19.293		0.497	1.00 37.89	8
	MOTA	621	0	LEU B 341				1.00 33.29	7
40	MOTA	622		LYS B 342	-18.003				6
	MOTA	623		LYS B 342	-16.737				6
	MOTA	624		LYS B 342	-15.603				6
	ATOM	625		LYS B 342	-14.210				6
	MOTA	626		LYS B 342	-13.155				6
45		627		LYS B 342	-11.775				7
	MOTA	628		LYS B 342	-10.790				6
	MOTA	629) C	LYS B 342	-16.744				8
	ATOM	630) 0	LYS B 342	-16.725				7
	ATOM	63.1	. N	ASN B 343	-16.760				
50	ATOM	632	CA	ASN B 343	-16.762				6
	MOTA	633	3 CB	ASN B 343	-16.97				6
	ATOM	634		ASN B 343	-16.178				6
	ATOM	635		ASN B 343	-14.938	3 72.313		_	8
	ATOM	63		ASN B 343	-16.87	7 71.144	-4.259		
55		63		ASN B 343	-17.89	4 75.624	-3.547		
))	MOTA	638		ASN B 343	-17.83		-4.284		
	ATOM	63:		GLY B 344	-18.93				
	ATOM	64		GLY B 344	-20.10		301-2.709	1.00 39.25	6
	VION	04	0 021	J	108				

5	ATOM	641		GLY B		-19.8		77.636	-2.258		38.26.	6
	ATOM	642	0	GLY B	344	-20.7		78.501	-2.484	1.00		8
٠	MOTA	643		GLY B		-18.7		77.871	-1.619	1.00		7
	MOTA	644		GLY B		-18.4		79.209	-1.159		34.00	6
	MOTA	645	С		345	-17.8		79.298	0.230		38.64	6
10	MOTA	646	0	GLY B	345	-17.2		80.303	0.573		38.14	8
	MOTA	647	N		346	-18.0		78.266	1.041	1.00		7
	MOTA	648	CA	LEU B	346	-17.5		78.279	2.403		36.05	6
	MOTA	649	CB	LEU B	346	-18.3		77.256	3.269		35.72	6
	MOTA	650	CG	LEU B	346	-19.8		77.473	3.378		34.89	6
15	MOTA	651		LEU B	346	-20.3		76.678	4.554		44.09	6
	MOTA	652	CD2	LEU B	346	-20.0		78.937	3.612		34.84	6
	MOTA	653	С	LEU B	346	-16.0		78.018	2.445		33.52	6
	MOTA	654	0	LEU B	346	-15.3		78.387	3.394		35.58	8 7
	MOTA	655	N	GLY B	347	-15.		77.388	1.385		30.47	
20	MOTA	656	CA	GLY B	347	-14.		77.078	1.305		33.01	6
	MOTA	657	С	GLY B		-13.		76.214	2.477		30.72	6
	MOTA	658	0	GLY B		-14.		75.243	2.808		30.89	8
	MOTA	659	N	VAL B		-12.		76.585	3.087		31.30	7
	MOTA	660	CA	VAL B		-12.		75.867	4.227	1.00	31.27	6 6
25	MOTA	661	СВ	VAL B		-10.		76.609	4.817	1.00	31.66	6
	MOTA	662	CG1			-11.		77.974	5.360	1.00	20.19 24.77	6
	MOTA	663	CG2			-10.		75.786	5.905	1.00	33.84	6
	MOTA	664	С	VAL B		-13.		75.651	5.360	1.00	29.99	8
	ATOM	665	0	VAL B		-13.		74.707	6.153		33.31	7
30	MOTA	666	И	VAL B		-14.		76.518	5.449		33.31	6
	MOTA	667	CA	VAL B		-15.		76.339	6.483 6.476		32.59	6
	MOTA	668	CB	VAL E		-16.		77.393 76.979	7.399		33.68	6
	MOTA	669	CG1			-17.		78.703	6.959		32.30	6
~ ~	MOTA	670	CG2			-15. -15.		74.987	6.380		34.91	6
35	MOTA	671	С	VAL E		-15. -16.		74.359	7.394		33.73	8
	ATOM	672	0	VAL E		-16. -16.		74.507	5.176		32.81	7
	ATOM	673	N	SER E		-16.		73.215	5.100	1.00		6
	ATOM	674 675	CA CB	SER I		-16. -16.		72.697	3.684		24.95	6
40	ATOM ATOM	676	OG		3 350	-17.		71.502	3.644		23.16	8
40		677	C		3 350	-15		72.254	5.942		31.59	6
	MOTA MOTA	678			350		417	71.807	6.950		37.62	8
	ATOM	679			351		675	71.942	5.565		28.60	7
	MOTA	680			B 351		905	71.010	6.378		29.82	6
45	ATOM	681			B 351		.419	71.139	6.050		27.49	6
73	ATOM	682			в 351		.151	71.094	4.585		30.22	6
	MOTA	683		1 ASP			.013		3.954	1.00	32.61	8
	ATOM	684		2 ASP			.064		4.017	1.00	30.02	8
	MOTA	685			B 351		.176		7.861	1.00	30.63	6
50		686			B 351		. 458		8.681	1.00	29.54	8
30	ATOM	687			в 352		.111		8.177		25.33	7
	ATOM	688			B 352		.346		9.533		28.59	6
	ATOM	689			в 352		.252		9.572		20.95	6
	ATOM	690			B 352		. 690				29.69	6
55		691			B 352		.757				30.36	8
,,,	ATOM	692			в 353		.754				27.63	7
	ATOM	693			В 353		.096				27.55	6
	ATOM	694			в 353		.144			1.00	28.04	6
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5	ATOM	695	CG2	ILE	В	353	-20.529	72.673	9.195	1 00	23.68	6
	MOTA	696	CG1			353	-19.108	74.657	8.869		27.33	6
	ATOM	697	CD1	ILE		353	-20.141	75.313	7.964		26.23	6
	MOTA	698	С	ILE	В	353	-18.309	71.002	9.775		30.88	6
	ATOM	699	0			353	-19.021	70.499	10.639		31.22	
10	MOTA	700	N	PHE		354	-17.728	70.279	8.822		29.86	8 7
	MOTA	701	ÇA	PHE		354	-17.881	68.831	8.797		31.08	
	ATOM	702	CB			354	-17.461	68.249	7.439		28.80	6
	MOTA	703	CG	PHE		354	-18.568	68.233	6.405		28.80	6
	ATOM	704	CD1	PHE		354	-19.031	69.403	5.833	1.00		6
15	MOTA	705	CD2			354	-19.150	67.027	6.034		29.45	6
	MOTA	706	CE1	PHE			-20.066	69.362	4.902		29.45	6
	ATOM	707	CE2			354	-20.186	66.978	5.104		25.19	6
	ATOM	708	CZ	PHE		354	-20.644	68.146	4.535	1.00		6
	MOTA	709	С	PHE		354	-17.041	68.223	9.913	1.00	_	6
20	ATOM	710	0	PHE	В	354	-17.544	67.429	10.700	1.00		6
	MOTA	711	N	ASP		355	-15.761	68.593	9.972		23.86	8
	MOTA	712	CA	ASP			-14.864		11.005		25.34	7
	MOTA	713	CB	ASP			-13.582	68.929	11.005		25.34	6
	MOTA	714	CG	ASP		355	-12.548	68.456	10.086		32.08	6
25	MOTA	715	OD1	ASP		355	-12.899	68.069	8.944			6
	MOTA	716	OD2	ASP		355	-11.345	68.477	10.450		33.58	8
	MOTA	717	С	ASP		355	-15.570	68.153	12.357		33.20	8
	ATOM	718	Ō	ASP		355	-15.430	67.257	13.182		27.86	6
	ATOM	719	N	LEU		356	-16.339	69.223	12.561		32.42	8
30	MOTA	720	CA	LEU		356	-17.085	69.400	13.803		26.84 28.66	7
	ATOM	721	СВ	LEU		356	-17.832	70.742	13.800		25.37	6
	ATOM	722	CG		В	356	-18.655	71.091	15.023		27.61	6
	ATOM	723	CD1		В	356	-17.729	71.248	16.191		25.43	6
	ATOM	724	CD2	LEU		356	-19.430	72.363	14.808		27.49	6
35	ATOM	725	С	LEU	В	356	-18.084	68.260	13.883		30.44	6 6
	ATOM	726	0	LEU	В	356	-18.054	67.445	14.804			8
	ATOM	727	N	GLY	В	357	-18.972	68.214	12.891		32.69	7
	MOTA	728	CA	GLY	В	357	-20.001	67.186	12.846	1.00		6
	ATOM	729	С	GLY	В	357	-19.486	65.832	13.279		33.12	6
40	ATOM	730	0	GLY	В	357	-20.032	65.246	14.207			8
	MOTA	731	N	MET	В	358	-18.444	65.351	12.593		33.31	7
	ATOM	732	CA	MET	В	358	-17.834	64.066	12.902		35.87	6
	ATOM	733	CB	MET	В	358	-16.513	63.903	12.151		34.56	6
	MOTA	734	CG	MET	В	358	-16.649	63.908	10.657		46.43	6
45	MOTA	735	SD	MET	В	358	-15.094	63.597	9.751		42.13	16
	ATOM	736	CE	MET	В	358	-14.121	65.063	10.228		44.29	6
	MOTA	737	С	MET	В	358	-17.552	63.976	14.392		33.26	6
	MOTA	738	0	MET	В	358	-18.019	63.075	15.075		36.39	8
	MOTA	739	N	SER	В	359	-16.766	64.933	14.875		33.31	7
50	MOTA	740	CA	SER	В	359	-16.380	64.998	16.270		34.39	6
	MOTA	741	CB	SER	В	359	-15.724	66.339	16.541		30.84	6
	ATOM	742	OG	SER	В	359	-15.130	66.355	17.825		47.14	8
	ATOM	743	С	SER	В	359	-17.579	64.813	17.169		36.43	6
	ATOM	744	0	SER	В	359	-17.635	63.853	17.922		35.46	8
55	ATOM	745	N	LEU			-18.525	65.744	17.079		36.74	7
	MOTA	746		LEU			-19.741	65.729	17.889		35.44	6
	ATOM	747		LEU			-20.706	66.817	17.405		34.16	6
	MOTA	748	CG	LEU	В	360	-20.263	68.255	17.575		34.59	6
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_		740 CD1	LEU B 360		05		,, , , , , , , , , , , , , , , , , , , ,	6 6
5	MOTA			-19.869			• • • • • • • • • • • • • • • • • • • •	
	MOTA		LEU B 360	-20.464				6
	MOTA	751 C		-21.021	64.011 18		· · · ·	8
	MOTA	752 0		-20.466		5.791 1.	00 40.96	7
	ATOM	753 N	SER B 361	-21.106			00 45.67	6
10	MOTA	754 CA	SER B 361	-20.532	61.630 15		00 46.45	6
	MOTA	755 CB	SER B 361			4.322 1.	00 51.81	8
	MOTA	756 OG	SER B 361	-20.750			00 44.49	6
	MOTA	757 C	SER B 361	-20.895			.00 46.67	8
	ATOM	758 0	SER B 361	-21.696			.00 41.44	7
15	MOTA	759 N	SER B 362	-19.811	Q		.00 42.13	6
13	MOTA	760 CA	SER B 362	-19.453	02.0		.00 42.61	6
	MOTA	761 CB	SER B 362	-17.962		•	,00 51.87	8
	MOTA	762 OG	SER B 362	-17.164	01.0		.00 38.41	6
		762 C	SER B 362	-20.228	~ - ·		.00 38.01	8
20	ATOM	764 0	SER B 362	-20.602			.00 34.55	7
20	MOTA	765 N	PHE B 363	-20.455	JJ			6
	ATOM	765 CA	262	-21.150	• • • •		.00 32.96	6
	ATOM		- 262	-21.006			00 31.99	6
	MOTA		,	-19.578			.00 29.97	6
	MOTA	,	o1 PHE B 363	-19.286			1.00 30.61	6
25	MOTA			-18.536			1.00 32.02	6
	MOTA	• • -	E1 PHE B 363	-17.966	•		1.00 33.67	
	MOTA		E2 PHE B 363	-17.221	65.222		1.00 30.91	6
	MOTA	, . –		-16.927	66.557		1.00 29.33	6
	MOTA	773 C	- 262	-22.617			1.00 30.52	6
30		774 C	262	-23.142			1.00 32.19	8
	MOTA	775 0	264	-23.279			1.00 33.51	7
	MOTA	776 N	0.51	-24.683			1.00.38.03	6
	MOTA			-24.855		22.111	1.00.42.32	6
	ATOM	•		-24.008		21.524	1.00 53.11	6
35				-24.183		20.344	1.00 59.51	8
	MOTA	,		-23.10		22.325	1.00 55.95	7
	MOTA		ND2 ASN B 364 ASN B 364	-25.49		22.091	1.00 31.89	6
	MOTA			-26.27		22.990	1.00 30.28	8
	MOTA		O ASN B 364 N LEU B 365	-25.30		21.673	1.00 27.62	7
4	MOTA 0			-26.00	•	22.280	1.00 29.36	6
	MOTA		CA LEU B 365	-25.40		21.743	1.00 27.54	6
	MOTA		CB LEU B 365	-23.89		21.738	1.00 38.91	6
	MOTA		CG LEU B 365	-23.39		21.190	1.00 34.47	6
	MOTA		CD1 LEU B 365	-23.39		23.143	1.00 34.24	
4	5 ATOM		CD2 LEU B 365	-27.49	_	21.987	1.00 26.23	
	ATOM	790	C LEU B 365	-27.93		20.863	1.00 27.06	
	ATOM	791	O LEU B 365	-28.29		23.022	1.00 25.23	7
	ATOM	792	N ASP B 366		-	22.878	1.00 26.07	6
	MOTA	1 793	CA ASP B 366	-29.7		24.076	1.00 29.68	
4	OTA 05		CB ASP B 366	-30.4			1.00 35.74	
•	ATO		CG ASP B 366	-30.2			1.00 36.78	
	ATO		OD1 ASP B 366	-30.2	-		1.00 41.23	
	ATO		OD2 ASP B 366	-30.0			1.00 27.70	
	ATO		C ASP B 366	-30.2			1.00 31.9	
	55 ATO		O ASP B 366					
	ATO		N ASP B 367	-31.4				
	OTA	·	CA ASP B 367	-32.0				
	OTA	_	CB ASP B 367	-33.5			1.00 30.0	
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5	ATOM	803	CG	700	D 267	.	· · · · · · · · · · · · · · · · · · ·	61 of 1 of 1		
•	ATOM	804		ASP :	B 367	-34.172		~ 2Y.081		6
	ATOM	805	OD2			-34.051				8
	MOTA	806	C		B 367	-34.829				8
	ATOM	807	0		B 367	-31.496			1.00 33.71	6
10	ATOM	808	И		B 367	-30.791			1.00 38.30	8
	ATOM	809	-	THR		-31.858		– – •		7
	ATOM	810	CA	THR I		-31.453			1.00 26.28	6
	ATOM	811	CB	THR 1		-31.567		26.643	1.00 27.30	6
	ATOM	812	OGI	_	=	-32.916		26.824	1.00 33.42	8
15	ATOM	813	CG2			-31.143		27.824	1.00 25.16	6
	ATOM	814	C	THR I		-30.025		25.181	1.00 21.13	6
	ATOM	815	0	THR I		-29.746		25.150	1.00 23.17	8
	ATOM	816	N		3. 369	-29.123		25.072		7
	ATOM		CA	GLU I		-27.711		24.932		6
20	MOTA	817 818	CB	GLU E		-26.947		24.878	1.00 32.79	6
20	ATOM	819	CG	GLU I		-27.229	-	26.130	1.00 36.29	6
	ATOM		CD	GLU E		-26.689	67.051	26.083	1.00 41.03	6
	ATOM	820	OE1			-26.960	66.318	25.102	1.00 42.05	8
	ATOM	821	OE2			-25.992	66.645	27.048	1.00 42.03	8
25	ATOM	822 823	C	GLU E		-27.428	71.527	23.731	1.00 25.57	6
23	ATOM		0	GLU E		-26.780	72.549	23.886	1.00 20.56	8
	ATOM	824 825	N	VAL E		-27.922	71.154	22.548	1.00 25.39	7
	ATOM		CA	VAL E		-27.710	71.968	21.355	1.00 25.99	6
	ATOM	826 827	CB	VAL E		-28.457	71.429	20.130	1.00 26.15	6
30	ATOM	828	CG1			-28.255	72.358	18.953	1.00 27.65	6
50	ATOM	829	CG2	_		-28.014	70.021	19.788	1.00 17.70	6
	ATOM	830	C	VAL E		-28.238	73.346	21.676	1.00 26.49	6
	ATOM	831	0	VAL E		-27.580	74.351	21.445	1.00 28.16	8
	ATOM	832	N	ALA B		-29.450	73.362	22.213	1.00 21.01	7
35	MOTA	833	CA	ALA B		-30.145	74.589	22.573	1.00 19.57	6
	ATOM	834	CB C	ALA B		-31.414	74.246	23.335	1.00 18.62	6
	ATOM	835		ALA B		-29.256	75.501	23.401	1.00 23.48	6
	ATOM	836	O N	ALA B		-28.936	76.613	22.989	1.00 32.67	8
	ATOM	837	CA	LEU B		-28.860	75.008	24.571	1.00 22.89	7
40	ATOM	838	CB			-27.999	75.758	25.472	1.00 23.28	6
	ATOM	839	CG	LEU B		-27.606	74.860	26.658	1.00 27.76	6
	ATOM	840		LEU B		-28.728	74.524	27.619	1.00 21.18	6
	ATOM	841		LEU B		-28.272	73.529	28.648	1.00 27.64	6
	ATOM	842	CDZ	TEO B		-29.198	75.801	28.284	1.00 20.90	6
45	ATOM	843	0	LEU B		-26.769	76.268	24.722	1.00 21.34	6
	ATOM	844	N	LEU B		-26.439	77.454	24.762	1.00 23.16	8
	ATOM	845	CA	LEU B		-26.111	75.349	24.023	1.00 24.42	7
	ATOM	846	CB			-24.916	75.669	23.254	1.00 23.78	6
	ATOM	847	CG	LEU B		-24.525	74.446	22.396	1.00 22.18	6
50	ATOM	848		LEU B		-23.098	74.283	21.942	1.00 31.52	6
	ATOM	849	CD1	LEU B		-22.196	74.576	23.100	1.00 31.93	6
	ATOM	850	C			-22.873	72.889	21.457	1.00 30.24	6
	ATOM	851	0	LEU B		-25.235	76.902	22.405	1.00 25.69	6
	ATOM	852	N	GLN B		-24.491	77.880	22.416	1.00 30.13	8
55	ATOM	853	CA	GLN B		-26.368	76.842	21.707	1.00 26.24	7
	ATOM	854		GLN B		-26.836	77.922	20.839	1.00 21.60	6
	ATOM	855		GLN B		-28.196	77.571	20.221	1.00 24.57	6
	ATOM	856	CD	GLN B		-28.188	76.330	19.348	1.00 21.02	6
				מ אורי	3/4	-29.538	76.071	18.698	1.00 22.86	6
						112				

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_		857 OE1 GLN B 374	-29.720 75.049 18.009 1.00 24.07 8
5	ATOM		-30.473 76.980 18.901 1.00 25.59 7
	MOTA		-26.988 79.249 21.569 1.00 20.66 6
	MOTA	- 054	-26.733 80.307 20.994 1.00 24.47 8
	MOTA	000 0 0===	-27.429 79.182 22.825 1.00 16.26
	MOTA	001 1	-27.639 80.374 23.631 1.00 17.16 6
10	MOTA	002 01. 1	-28.435 80.025 24.865 1.00 19.53 6
	MOTA	000 05	-26 304 80.966 24.025 1.00 25.13 6
	MOTA	004 0	-26 074 82.154 23.833 1.00 23.81 8
	MOTA	865 O ALA B 375	-25 433 80.111 24.568 1.00 24.57 7
	MOTA	866 N VAL B 376	-24 102 80 526 24.986 1.00 25.80 6
15	MOTA	867 CA VAL B 376	_23 192 79 321 25.234 1.00 26.48 6
	MOTA	868 CB VAL B 376	-21.806 79.780 25.620 1.00 23.20 6
	MOTA	869 CG1 VAL B 376	-23.771 78.433 26.310 1.00 19.08 6
	MOTA	870 CG2 VAL B 376	-23.510 81.403 23.898 1.00 25.69 6
	MOTA	871 C VAL B 376	-23.510 81.465 24.166 1.00 27.87 8 -22.796 82.364 24.166 1.00 27.87 8
20	MOTA	872 O VAL B 376	7 1 22 1 20 23 09 7
	MOTA	873 N LEU B 377	-23.827 01.013 22 06 6
	MOTA	874 CA LEU B 377	-23.340. 01.77
	MOTA	875 CB LEU B 377	-23.552 60.525 20.516 1.00.22 65 6
	MOTA	876 CG LEU B 377	222.750 75.000 2.00 16.70 6
25	MOTA	877 CD1 LEU B 377	-23.221 70.700 10.000 10.58 6
	MOTA	878 CD2 LEU B 377	-21.300 79.333 20.36 14 6
	MOTA	879 C LEU B 377	-24.075 03.101 1.00 20 62
	MOTA	880 O LEU B 377	-23.464 64.104 21.00 28 99 7
	MOTA	881 N LEU B 378	-25.390 05.025 147 1 00 29 87 6
30	MOTA	882 CA LEU B 378	-20.220 04.24.
	MOTA	883 CB LEU B 378	-27.090 03.034 21.000 1 00 20 03 6
	MOTA	884 CG LEU B 378	-28.040 03.005 1 00 27 97 6
	MOTA	885 CD1 LEU B 378	-28.507 03.001 100 1 00 27 69 6
	MOTA	886 CD2 LEU B 378	-30.072 84.605 21.692 1.00 27.69 -25.738 85.280 22.090 1.00 31.09 6
35	MOTA	887 C LEU B 378	-25.738 86.379 21.651 1.00 31.77 8
	MOTA	888 O LEU B 378	-25.695 84.931 23.376 1.00 31.44 7
	MOTA	889 N MET B 379	-25.291 85.851 24.434 1.00 32.62 6
	MOTA	890 CA MET B 379	-25.797 85.335 25.793 1.00 31.45 6
	MOTA	891 CB MET B 379	-27.332 85.262 25.883 1.00 38.75 6
4(MOTA (892 CG MET B 379	-28.020 86.915 25.550 1.00 41.27 16
	MOTA	893 SD MET B 379	-29.814 86.586 25.513 1.00 35.68 6
	MOTA	894 CE MET B 379	-23.796 86.129 24.538 1.00 33.72 6
	MOTA	895 C MET B 379	-23.246 86.190 25.633 1.00 36.29 8
	MOTA	896 O MET B 379	-23.240 00.230 1 00 34 49 7
4	5 ATOM	897 N SER B 380	-23.132 00.33 97 6
	ATOM	898 CA SER B 380	-21.730 00.000 1 00 31 24 6
	MOTA		-21.132 00.300 - 1.00.30 42 8
	MOTA		-21.224 01.310 1 00 30 69 6
	MOTA		-21.033 00.110 1 00 44 64 8
5	MOTA 0	902 O SER B 380	-22.004 00.303 1 00 41 04 7
	MOTA	903 N SER B 381	221.035 00:101 1 00 44 91 6
	MOTA	904 CA SER B 381	220.907 03.020 200 44.50 6
	ATOM	905 CB SER B 381	-20.610 89.832 26.737 1 20 45 42 8
	ATOM	1 906 OG SER B 381	-19.351 69.223 21.600 1 00 44 59 6
	55 ATOM	1 907 C SER B 381	-19.815 90.014 24.002 1 00 40 32 8
•	ATON	1 908 O SER B 381	-19.725 91.023 21.02 3 00 43 75 7
	ATON	1 909 N ASP B 382	-18.977 89.922 23.010 1.00 43.93 6
	ATO		-17.886 90.556 23.144 1:00 2000
			113

5	ATOM .	911	CB	ASP	В	382	-16.727	89.562	23.028	1.00	48.39	6
	MOTA	912	CG	ASP	В	382	-17.142	88.232	22.471	1.00	53.23	6
	ATOM	913	OD1		В	382	-18.102	87.621	23.002	1.00	56.97	8
	ATOM	914	OD2	ASP		382	-16.513	87.753	21.480	1.00	58.91	
	ATOM	915	C		В	382	-18.191					8
10	ATOM	916						91.172	21.772	1.00		6
10			0	ASP		382	-17.366	91.899	21.229	1.00	40.93	8
	ATOM	917	N	ARG		383	-19.369	90.908	. 21.224	1.00	42.63	7
	MOTA	918	CA	ARG		383	-19.698	91.445	19.934	1.00	43.32	6
	ATOM	919	CB	ARG		383	-21.131	91.101	19.557	1.00	42.31	6
	MOTA	920	ÇG	ARG		383	-21.619	89.672	19.811	1.00	40.83	6
15	MOTA	921	CD	ARG	В	383	-21.144	88.627	18.804	1.00	38.09	6
	MOTA	922	NE	ARG	В	383	-21.922	87.415	18.943	1.00	37.33	7
	ATOM	923	CZ	ARG	В	383	-21.584	86.250	18.411	1.00	38.35	6
	MOTA	924	NH1	ARG	В	383	-20.465	86.143	17.700	1.00	33.70	7
	MOTA	925	NH2	ARG	В	383	-22.369	85.196	18.604	1.00	35.46	, 7
20	ATOM	926	С	ARG		383	-19.591	92.958	20.007	1.00	44.96	6
	ATOM	927	0	ARG		383	-20.050	93.577	20.980	1.00	45.60	
	ATOM	928	N	PRO		384	-18.975	93.579	19.005	1.00		8
	ATOM	929	CD	PRO		384	-18.395				45.33	7
	ATOM	930	CA	PRO		384		92.881	17.854	1.00	46.85	6
25	ATOM	931		PRO			-18.808	95.035	18.947	1.00	47.37	6
23			CB			384	-17.868	95.255	17.764	1.00	46.90	6
	MOTA	932	CG	PRO		384	-17.575	93.934	17.187	1.00	46.41	6
	ATOM	933	С	PRO		384	-20.125	95.778	18.762	1.00	48.29	6
	ATOM	934	0	PRO		384	-21.048	95.277	18.120	1.00	48.34	. 8
20	ATOM	935	N	GLY		385	-20.185	96.994	19.314	1.00	49.88	7
30	ATOM	936	CA	GLY		385	-21.371	97.838	19.192	1.00	50.35	6
	ATOM	937	С	${ t GLY}$		385	-22.410	97.615	20.265	1.00	50.70	6
	ATOM	938	0	\mathtt{GLY}	В	385	-23.382	98.363	20.374	1.00	53.48	8
	ATOM	939	N	LEU	В	386	-22.205	96.557	21.044	1.00	49.04	7
	MOTA	940	CA	LEU	В	386	-23.136	96.211	22.101	1.00	50.53	6
35	MOTA	941	CB	LEU	В	386	-22.640	94.972	22.853	1.00	45.17	6
	ATOM	942	CG	LEU	В	386	-22.744	93.653	22.121	1.00	48.26	6
	ATOM	943	CD1	LEU	В	386	-22.122	92.525	22.938	1.00	41.68	6
	ATOM	944	CD2	LEU	В	386	-24.215	93.376	21.852	1.00	38.40	6
	ATOM	945	С	LEU		386	-23.322	97.357	23.058	1.00	52.13	6
40	ATOM	946	0	LEU			-22.438	98.182	23.234		53.67	8
	ATOM	947	N	ALA			-24.499	97.398	23.666		53.42	7
	ATOM	948	CA	ALA			-24.830	98.441	24.624			
	ATOM	949	СВ	ALA			-26.223	98.993			56.01	6
	ATOM	950	C	ALA			-24.775		24.339		56.47	6
45	MOTA	951	0	ALA				97.853	26.024		55.52	6
15	ATOM	952					-23.798	98.027	26.753		53.75	8
			N	CYS			-25.843	97.145	26.371		56.03	7
	ATOM	953	CA	CYS			-26.000	96.525	27.673		59.57	6
	ATOM	954	CB	CYS			-27.469	96.134	27.839		59.23	6
50	MOTA	955	SG	CYS			-28.620	97.392	27.264	1.00	58.64	16
50	MOTA	956	С	CYS			-25.105	95.283	27.798	1.00	62.18	6
	ATOM	957	0	CYS	В	388	-25.590	94.164	27.868	1.00	67.88	8
	ATOM	958	N	VAL	В	389	-23.789	95.510	27.824	1.00	60.78	7
	MOTA	959	CA	VAL	В	389	-22.797	94.434	27.959		57.70	6
	MOTA	960	CB	VAL	В	389	-21.355	94.976	27.998		57.09	6
55	ATOM	961	CG1				-20.361	93.832	28.085		59.03	6
	MOTA	962	CG2				-21.065	95.845	26.791		53.98	6
	ATOM	963	C	VAL			-23.078	93.642	29.230		57.77	6
	ATOM	964	Ö	VAL			-23.727	92.602	29.230		60.94	8
	. =	•	-		_		111	22.002	29.203	1.00	00.94	σ

	110 33.5		• •
_		965 N ALA B 390	-22.561 94.159 30.332 1.00 52.68 7
5	ATOM	966 CA ALA B 390	-22.684 93.570 31.655 1.66
	MOTA	967 CB ALA B 390	-22.650 94.681 32.710
	MOTA	907 02 1221 -	-23.905 92.697 31.077 1.00 51 05
	MOTA	900 0 1221 -	-23.784 91.576 32.369 1.00 51.95
	MOTA	909 0 1221 -	-25.075 93.216 31.498 1.00 47.11
10	MOTA	970 21 122.2	00 220 02 481 31.656 1.00 51.04
	MOTA	3/1 011 1111	27 502 93 318 31.122 1.00 54.22 6
	MOTA	972 CB ARG B 391	20 007 02 713 31.430 1.00 64.20 6
	MOTA	973 CG ARG B 391	30.059 93.582 30.929 1.00 73.80 6
	MOTA	974 CD ARG B 391	21 361 93 097 31.378 1.00 79.76 7
15	ATOM	975 NE ARG B 391	21 736 93 015 32 656 1.00 84.27 6
	MOTA	976 CZ ARG B 391	7 1 100 95 28
	ATOM	977 NH1 ARG B 391	-30.867 93.372 00.055 1.00.86.84 7
	MOTA	978 NH2 ARG B 391	-32.957 92.555 20.040 1.00 48 18 6
	ATOM	979 C ARG B 391	-26.277 91.133 31.465 1.00 49 57 8
20	ATOM	980 O ARG B 391	-26.724 90.113 00 45 01 7
20	ATOM	981 N ILE B 392	-25.743 91.167 29.718 1.00 18.77 6
		982 CA ILE B 392	-25.592 89.999 28.807 1.00 46 45 6
	ATOM	983 CB ILE B 392	-25.112 90.424 27.405 1.00 10 35
	MOTA	984 CG2 ILE B 392	-24.805 89.221 26.614 1.00 40.60
	ATOM	985 CG1 ILE B 392	-26.178 91.283 26.766 1.00 51.00 6
25	MOTA	986 CD1 ILE B 392	-25.762 91.768 25.366 1.00 50 90 6
	MOTA	200	-24.671 88.935 29.462 1.00 50.21
	MOTA	307 0 224	-25.086 87.780 29.803 1.00 0.00
	MOTA	900 0 === = 202	-23.431 89.298 29.790 1.00 50.43
	MOTA	905 11 000	-22.504 88.328 30.378 1.00 50.30 6
30		990 011 020 -	-21.314 89.022 31.044 1.00 53.97
	MOTA	991 02 02-	-20.063 89.005 30.209 1.00 62.16
	MOTA	202	-18.877 89.415 30.976 1.00 67.69
	MOTA	995 05 020	-17.709 89.264 30.656 1.00 66.42
	ATOM	- 202	-18.897 89.976 32.052 1.00 70.64 8
35	MOTA 5	995 OE2 GLU B 393	-23.251 87.477 31.416 1.00 49.51
	MOTA	990 0 0 0	-23.226 86.260 31.303 1.00 49.33
	MOTA	201	_23 898 88.153 32.409 1.00 46.07
	MOTA	950 11 ===	24 721 87 579 33.506 1.00 45.76
	MOTA	999 CA LYS B 394	25 594 88 693 34.161 1.00 43.85
4	MOTA 0		25.626 86 548 32.851 1.00 46.69 6
	MOTA ·		25.772 85 430 33.329 1.00 49.13 8
	ATOM		26 203 86 948 31.719 1.00 46.57
	MOTA		27 076 86 078 30.938 1.00 43.33 6
	ATOM		27 621 86 821 29.716 1.00 48.44 6
4	45 ATOM	1 1005 CB TYR B 395	20 927 87 688 29.980 1.00 53.83 6
	MOTA	1 1006 CG TYR B 395	20.52
	MOTA	$_{ m 4}$ 1007 CD1 TYR B 395	22 221 90 469 29 309 1.00 59.73 6
	MOTA	4 1008 CE1 TYR B 395	-30.531 69.405 251113 1.00 56.47 6
	IOTA	M 1009 CD2 TYR B 395	-29.596 67.505 52.12
	50 ATO	M 1010 CE2 TYR B 395	30.723 00.233 30.446 1.00 63.18 6
	ATO		-31.090 03.202 1 200 64 46 8
	ATO	20 myn p 30s	32.189 90.000 30.071 2.00 37 30 6
		201 G WAD B 301	5 -26.276 84.867 30.403 1.00 34 10 8
	OTA	20 myp D 301	5 -26.611 83.737 30.825 1.00 31 92 7
	ATO		6 -25.213 85.108 29.710 1.00 24 81 6
	55 ATO	22 CTN D 30	6 -24.380 84.018 29.244 1.00 34.61 6
	ATC	GTN B 30	6 -23.176 84.550 28.464 1.00 32.04
	ATC	TO CIN P 30	
	ATO	DM 1018 CG GLN B 39	115

5	ATOM	1019	CD	GLN	В	396	-21.214	83.871	27.016	1.00 29.46	6
	MOTA	1020	OE1	GLN	В	396	-20.547	84.930	27.109	1.00 34.65	_
	ATOM	1021	NE2	GLN	В	396	-21.112	83.032	25.992	1.00 27.21	-
	MOTA	1022	С	GLN	В	396	-23.908	83.207	30.434	1.00 37.13	
	MOTA	1023	0	GLN	В	396	-23.876	81.986	30.384	1.00 37.36	
10	MOTA	1024	N	ASP	В	397	-23.544	83.903	31.508	1.00 38.61	
	ATOM	1025	CA		В	397	-23.069	83.250	32.717	1.00 40.37	
	MOTA	1026	СВ	ASP		397	-22.617	84.297	33.754	1.00 40.51	
	MOTA	1027	CG	ASP		397	-21.360	85.025	33.352	1.00 43.77	
	MOTA	1028	OD1	ASP		397	-20.337	84.366	33.054	1.00 46.50	
15	MOTA	1029			В	397	-21.343	86.287	33.350	1.00 51.34	
	MOTA	1030	С	ASP	В	397	-24.223	82.422	33.267	1.00 38.62	
	MOTA	1031	0	ASP		397	-24.023	81.327	33.778	1.00 39.20	
	ATOM	1032	N	SER		398	-25.432	82.962	33.138	1.00 37.84	
	MOTA	1033	CA	SER		398	-26.633	82.293	33.622	1.00 37.80	
20	MOTA	1034	CB	SER		398	-27.830	83.246	33.501	1.00 34.28	
	ATOM	1035	OG	SER		398	-28.995	82.715	34.114	1.00 46.60	
	ATOM	1036	С	SER	В	398	-26.911	80.997	32.867	1.00 38.41	
	ATOM	1037	0	SER	В	398	-27.454	80.047	33.433	1.00 39.98	
	ATOM	1038	N	PHE	В	399	-26.546	80.963	31.587	1.00 34.82	
25	ATOM	1039	CA	PHE	В	399	-26.772	79.768	30.781	1.00 35.96	
	MOTA	1040	CB	PHE	В	399	-26.892	80.100	29.293	1.00 35.75	
	ATOM	1041	CG	PHE	В	399	-28.211	80.717	28.906	1.00 39.30	
	MOTA	1042	CD1	PHE	В	399	-28.466	82.056	29.109	1.00 39.86	
	ATOM	1043	CD2	PHE	В	399	-29.194	79.938	28.355	1.00 36.81	
30	ATOM	1044	CE1	PHE	В	399	-29.700	82.602	28.739	1.00 41.25	
	MOTA	1045	CE2	PHE	В	399	-30.424	80.483	27.987	1.00 43.61	
	MOTA	1046	CZ	PHE	В	399	-30.677	81.813	28.181	1.00 40.34	6
	MOTA	1047	С		В	399	-25.658	78.754	30.976	1.00 33.48	6
~ ~	MOTA	1048	0		В	399	-25.927	77.589	31.256	1.00 26.86	8
35	MOTA	1049	N	LEU		400	-24.408	79.187	30.796	1.00 31.47	7
	MOTA	1050	CA	LEU		400	-23.275	78.291	30.945	1.00 37.41	. 6
	MOTA	1051	CB	LEU		400	-21.976	79.091	31.030	1.00 34.24	6
	ATOM	1052	CG	LEU		400	-21.470	79.642	29.726	1.00 35.10	
40	ATOM	1053	CD1	LEU		400		80.304	29.917	1.00 26.60	6
40	MOTA	1054		LEU		400	-21.326	78.488	28.759	1.00 29.44	6
	ATOM	1055	С	LEU			-23.430	77.376	32.145	1.00 38.84	
	ATOM	1056	0			400		76.157	32.007	1.00 40.38	
	ATOM	1057	N	LEU			-23.639	77.968	33.321	1.00 42.79	
45	ATOM	1058	CA	LEU			-23.801	77.181	34.537	1.00 43.48	
43	MOTA	1059	CB	LEU			-24.226	78.067	35.712	1.00 44.73	
	ATOM	1060	CG	LEU			-24.378	77.303	37.012	1.00 51.39	
	ATOM	1061		LEU			-22.990	76.844	37.484	1.00 50.11	
	ATOM	1062		LEU			-25.027	78.163	38.083	1.00 49.30	
50	ATOM	1063	С	LEU			-24.854	76.095	34.311	1.00 41.62	
50	ATOM	1064	0	LEU			-24.576	74.900	34.427	1.00 45.14	
	MOTA	1065	N	ALA			-26.068	76.532	33.997	1.00 37.92	
	ATOM	1066	CA	ALA			-27.177	75.631	33.752	1.00 29.90	
	MOTA	1067	CB	ALA			-28.361	76.433	33.200	1.00 30.70	
55	ATOM	1068	C	ALA			-26.779	74.521	32.773	1.00 28.88	6
رر	ATOM	1069	O N	ALA			-27.078	73.347	32.996	1.00 32.14	8
	ATOM	1070	N	PHE			-26.091	74.908	31.698	1.00 31.07	
	ATOM	1071 1072	CA	PHE			-25.655	73.970	30.673	1.00 29.90	
	MOTA	10/2	СВ	PHE	B	403	-24.847	74.715	29.607	1.00 27.03	6
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_	2 EIOM	1073	CG F	HE B 403	-24.55			35 59- 1	900.2 0 5	55 6	
5	ATOM	1074		HE B 403	-23.91			_	.00 25.		
	ATOM	1074	CD2 F		-24.93				.00 19.		
	MOTA			PHE B 403	-23.6				1.00 27.		
	MOTA	1076		PHE B 403	-24.6				1.00 22.		
	MOTA	1077		PHE B 403	-24.0		.439		1.00 22.		
10	MOTA	1078			-24.8		.902		1.00 28.	-	5
	MOTA	1079			-25.0		.726		1.00 26.		3
	MOTA	1080			-23.7		.335	32.037	1.00 30.		7
	MOTA	1081		GLU B 404	-22.8		.419	32.712	1.00 34.	.03	6
	MOTA	1082		GLU B 404	-21.8		3.215	33.527	1.00 39.	. 45	6
15	MOTA	1083		GLU B 404	-21.6	_	2.384	34.068	1.00 47	. 68	6
	MOTA	1084		GLU B 404	-19.		3.129	34.996	1.00 54	.02	6
	MOTA	1085	CD	GLU B 404			4.290	34.701	1.00 57		8
	MOTA	1086	OE1	GLU B 404	-19.3		2.555	36.048	1.00 63		8
	MOTA	1087	OE2	GLU B 404	-19.3		1.509	33.642	1.00 36		6
20	MOTA	1088	С	GLU B 404	-23.	-		33.640		.64	8
20	MOTA	1089	0	GLU B 404	-23.	_	0.292	34.458	1.00 29		7
	MOTA	1090	N	HIS B 405	-24.		2.131	35.405	1.00 31		6
	MOTA	1091	CA	HIS B 405	-25.	_	1.387	36.173	1.00 33		6
	ATOM	1092	CB	HIS B 405	-26.		2.324	37.163	1.00 34		6
25	MOTA	1093	CG	HIS B 405	-25.		3.185	37.103	1.00 34		6
23	ATOM	1094		HIS B 405	-24.		3.286	37.969	1.00 32		7
	ATOM	1095	ND1	. HIS B 405	-26.		74.101	38.769	1.00 36		6
	MOTA	1096	CE1	. HIS B 405	-25.		74.703	38.511	1.00 39		7
	ATOM	1097		HIS B 405	-24		74.222	34.648	1.00 3		6
30		1098		HIS B 405			70.342	35.006	1.00 3		8
50	ATOM	109		HIS B 405			69.160		1.00 3		7
	MOTA			TYR B 406			70.776		1.00 2		6
	MOTA	_		TYR B 406			69.853			1.48	6
	ATOM			TYR B 406			70.537		1.00 2		6
35				TYR B 406			69.576		1.00 1		6
55	ATOM			1 TYR B 400		.179	69.047		1.00 2		6
	MOTA		5 CE	1 TYR B 40	-	.893	68.128				6
	ATOM			2 TYR B 40	-	.525	69.152				6
	ATOM			2 TYR B 40		.241	68.228				. 6
40						.420	67.713	_			8
-11	MOTA			TYR B 40		120	66.802				6
	ATON			TYR B 40		5.697	68.72			27 08	8
	ATO			TYR B 40		7.155	67.60			25 76	7
	ATO			ILE B 40		5.422	69.05				6
4	5 ATO			A ILE B 40		4.428	68.09				6
-	ATO					3.090	68.77				. 6
	ATO			G2 ILE B 40		1.959	67.77			43.30	6
	ATO			G1 ILE B 40		3.214	69.51			40.40	6
	ATO		17 C	D1 ILE B 40)7 –2	3.655	68.61			39.03	6
4	TO ATO	_	18 C			4.191	67.00			35.18	8
•	ATO		19 0	_)7 –2	4.178	65.80			37.25	7
	ATO		.20 N)8	3.990	67.42			37.23	6
	ATC			A ASN B 4	08 -2	3.739	66.47				6
	ATC	-		B ASN B 4		3.524	67.22			32.27	6
				G ASN B 4		2.296	68.13			33.56	
	55 ATC ATC			DD1 ASN B 4	08 -2	21.194	67.6			31.99	
	ATC	_	125 N	ND2 ASN B 4	08 -2	22.478	69.3			31.23	
	ATC ATC			ASN B 4	08 -:	24.876	65.4	53 35.03	56 I.UU	38.14	U
	ATC	Ot-1 T	`	- '		17					

•		WO 9	9/060014										1	PCT/US9	9/06899	
	5	ATOM	1127	0	ASN	В	408	_	24.6	24	64.253	35.	105	1.00	42.16	8
1		ATOM	1128	N	TYR	В	409	-	26.1	22	65.924	35.	.003	1.00	35.62	7
		ATOM	1129	CA	TYR	В	409	_	27.2	73	65.024	35.	.073	1.00	35.91	6
		MOTA	1130	СВ	TYR	В	409	_	28.5	97	65.787	34.	.931	1.00	34.41	6
		ATOM	1131	CG	TYR	В	409	_	29.7	88	64.868	34	. 685	1.00	38.73	6
	10	ATOM	1132	CD1	TYR	В	409	-	30.0	64	63.819	35	.549	1.00	41.34	6
		MOTA	1133	CE1	TYR	В	409	_	31.1	.30	62.962	35	.309	1.00	47.16	6
		MOTA	1134	CD2	TYR	В	409	-	30.6	313	65.037	33	.579	1.00	46.20	6
		MOTA	1135	CE2	TYR	В	409	-	31.6	84	64.176	33	.341	1.00	50.74	6
		MOTA	1136	CZ	TYR	В	409	-	31.9	42	63.143	34	.206	1.00	50.88	6
	15	ATOM	1137	OH	TYR	В	409	_	33.0	02	62.312	33	.978	1.00	53.14	8
		ATOM	1138	С	TYR	В	409	_	27.2	215	64.020	33	.951	1.00	38.16	6
		MOTA	1139	0	TYR	В	409	-	27.5	558	62.857	34	.111	1.00	41.83	8
		MOTA	1140	N	ARG	В	410	_	26.8	324	64.528	32	.796	1.00	42.25	7
		MOTA	1141	CA	ARG	В	410	-	26.7	734	63.739	31	.594	1.00	42.83	6
	20	MOTA	1142	CB	ARG		410	-	26.3	350	64.646	30	.441	1.00	36.83	6
		MOTA	1143	CG	ARG				27.4		65.585	29	.945		34.32	6
		MOTA	1144	CD	ARG				28.2		64.863		.917		36.62	6
		MOTA	1145	NE	ARG		410		27.4		64.378		.829		38.64	7
		ATOM	1146	CZ	ARG		410		27.9		63.656		.824		35.73	6
	25	MOTA	1147		ARG				29.2		63.379		.782		33.17	7
		MOTA	1148		ARG				27.0		63.227		.868		32.70	7
		MOTA	1149	С	ARG				25.6		62.664		.733		46.67	6
		MOTA	1150	0	ARG		410		25.8		61.547		.257		41.78	8
	20	ATOM	1151	N	LYS		411		-24.6		63.028		.413		52.99	7
	30	ATOM	1152	CA	LYS		411		-23.4		62.145		.609		58.32	6
		ATOM	1153	CB	LYS		411		-23.0		61.249		.833		64.99	6
		MOTA	1154	CG	LYS		411		-24.9		60.544 59.887		.968		70.48	6
		MOTA	1155 1156	CD CE	LYS LYS				-25.0 -26.2				.349		77.18 84.30	6
	35	ATOM ATOM	1156	NZ			411 411		-26.2		58.944 58.242		.474		86.48	6 7
	33	ATOM	1157	C			411		-23.		61.341		.365		56.66	6
		ATOM	1159	0			411		-23.		60.199		.210		55.47	8
		ATOM	1160	N			412		-22.		62.026		.479		54.67	7
		ATOM	1161	CA			412		-22.		61.474		.214		48.67	6
	40	ATOM	1162	CB			412		-21.		62.599		.310		43.14	6
		ATOM	1163	CG			412		-22.		63.501		.784		41.36	6
		ATOM	1164		HIS				-23.		64.603		.299		35.44	6
		ATOM	1165		HIS				-23.		63.290		.539		38.19	7
		ATOM	1166		HIS				-24.		64.238		.353		34.75	6
	45	ATOM	1167		HIS				-24.		65.034		.396		35.52	7
		MOTA	1168	С			412		-20.		60.596		.644		46.35	6
		MOTA	1169	0	HIS	В	412		-20.		60.892		.644		42.73	8
		MOTA	1170	N	HIS	В	413	-	-20.	708	59.469		.973	1.00	48.92	7
		MOTA	1171	CA	HIS	В	413		-19.	593	58.614		.371	1.00	53.15	6
	50	MOTA	1172	CB	HIS	В	413		-20.	022	57.147	29	.421	1.00	55.27	6
		MOTA	1173	CG	HIS	В	413	-	-20.	814	56.823	30	.636	1.00	58.77	6
		MOTA	1174	CD2	HIS	В	413		-22.	019	56.223	30	.822	1.00	61.65	6
		ATOM	1175	ND1	HIS	В	413		-20.	360	57.159		.921		60.31	7
		ATOM	1176	CE1	HIS	В	413		-21.		56.758		.809	1.00	63.01	6
	55	ATOM	1177	NE2	HIS	В	413		-22.		56.193		.171	1.00	62.93	7
		ATOM	1178	С	HIS	В	413		-18.	426	58.862	28	.438	1.00	53.19	6
		ATOM	1179	0			413	-	-17.	975	57.996	27	.699	1.00	54.93	8
		MOTA	1180	N	VAL	В	414	-	-17.	970	60.113	28	.521	1.00	53.77	7
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		03	CB 17	AL B 414	-16.845	60.674		00 51.06	6
5	MOTA	1181		AL B 414	-17.317	61.498		1.00 51.49	6
	MOTA	1182		AL B 414	-16.133	62.122		1.00 45.22	6
	MOTA	1183			-18.095	60.631		1.00 52.67	6
	MOTA	1184			-16.096	61.557	28.775	1.00 54.28	6
	MOTA	1185	_	AL B 414	-16.700	62.283	29.574	1.00 55.49	8
10	MOTA	1186		AL B 414	-14.770	61.466		1.00 56.28	7
	MOTA	1187		THR B 415	-13.919	62.234		1.00 57.83	6
	MOTA	1188		THR B 415	-12.488	61.686		1.00 59.64	6
	MOTA	1189		THR B 415		62.572		1.00 66.69	8
	MOTA	1190		THR B 415	-11.618	61.483	28.227	1.00 59.42	6
15	MOTA	1191		THR B 415	-11.988	63.726	29.352	1.00 56.98	6
	MOTA	1192		THR B 415	-13.840		28.216	1.00 55.70	8
	ATOM	1193		THR B 415	-13.987	64.135	30.387	1.00 57.44	7
	MOTA	1194		HIS B 416	-13.598	64.522	30.387	1.00 57.34	6
	MOTA	1195	CA	HIS B 416	-13.485	65.972	29.653	1.00 57.31	6
20	ATOM	1196	CB	HIS B 416	-12.114	66.326		1.00 69.78	6
20	ATOM	1197	CG	HIS B 416	-10.968	65.931	30.513	1.00 03.70	6
	ATOM	1198	CD2	HIS B 416	-9.930	65.082	30.307	1.00 71.42	7
	ATOM	1199	ND1	HIS B 416	-10.756	66.480	31.787	1.00 72.49	6
	ATOM	1200		HIS B 416	-9.631	65.973	32.281	1.00 73.30	7
25	MOTA	1201		HIS B 416	-9.120	65.131	31.408	1.00 73.91	6
23	MOTA	1202		HIS B 416	-14.560	66.515		1.00 52.81	8
	ATOM	1203		HIS B 416	-14.334			1.00 48.05	7
	ATOM	1204		PHE B 417	-15.746			1.00 47.99	6
	MOTA	1205		PHE B 417	-16.841				6
30	ATOM	1206		PHE B 417	-18.152			1.00 46.11	6
30	ATOM	120		PHE B 417	-19.233			1.00 44.27	6
	MOTA	1208			-19.280			1.00 41.79	6
	MOTA	120		PHE B 417	-20.118			1.00 40.23	6
	MOTA	121		. PHE B 417	-20.233			1.00 44.30	6
35		121		PHE B 417	-21.072		_	1.00 36.80	6
55	ATOM	121		PHE B 417	-21.119			1.00 40.69	6
	MOTA	121		PHE B 417	-17.020			1.00 46.69	8
	MOTA			PHE B 417	-16.79			1.00 43.35	7
	MOTA			TRP B 418	-17.44			1.00 45.14	6
40				TRP B 418	-17.68				6
40	ATOM ATOM			TRP B 418	-18.04				
	ATOM				-18.16				
	ATOM				-19.29				
	ATOM				-18.95				
4:				3 TRP B 418	-20.56				
7.	ATOM			1 TRP B 418	-17.22				
	ATOM				-17.69				
	OTA	_			-19.81				
	OTA			3 TRP B 418	-21.42				
5	OTA 0				-21.06				
,	OTA U		27 C	TRP B 418	-16.50	70.6			
			28 0	TRP B 418	-16.6	71 71.4			
	ATO		29 N	PRO B 419	-15.29				
	ATO	_	30 CI		-14.9	_			
	ATO		30 C		-14.1		23 29.01		
3	55 ATO		31 C	- 410	-12.9		82 29.72		
	OTA		32 C	- 440	-13.5		03 30.77		
	ATO	-		410	-14.0			9 1.00 36.2	8 6
	ATO	IM T	234 C	ETO D 273	119				
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5	MOTA	1235	0	PRO I	3 4	19	-1	3.690	72	.001	26.	754	1.00	37.08	8
	MOTA	1236	N	LYS 1	3 4	20	-1	4.330	69	.871	26.	976	1.00	35.96	7
	MOTA	1237	CA	LYS I	3 4	20	-1	4.278	69	.609	25.	538	1.00	40.82	6
	MOTA	1238	CB	LYS 1	3 4	20	-1	4.452	68	.103	25.	271	1.00	40.78	6
	ATOM	1239	CG	LYS I	3 4	20	-1	3.349	67	.214	25.	830	1.00	48.62	6
10	MOTA	1240	CD	LYS I	3 4	120	-1	3.565	65	.746	25.	480	1.00	55.12	6
	MOTA	1241	CE	LYS I	В 4	20	-1	2.427	64	.892	26.	017	1.00	53.26	6
	MOTA	1242	ΝZ	LYS I	B 4	20	-1	2.582	63	.457	25.	608	1.00	52.69	7
	MOTA	1243	С	LYS I	В 4	120	-1	5.414	70	.374	24.	875	1.00	40.29	6
	MOTA	1244	0	LYS I	B 4	120	-1	5.225	71	.015	23.	851	1.00	39.66	8
15	MOTA	1245	N	LEU :	В 4	121	-1	6.591	70	.300	25.	499	1.00	38.33	7
	ATOM	1246	CA	LEU :	В 4	121	-1	7.796	70	.958	25.	001	1.00	37.60	6
	MOTA	1247	CB	LEU :	В 4	121	-1	8.970	70	.702	25.	965	1.00	43.66	6
	MOTA	1248	CG	LEU :	В 4	121	-2	0.370	70	.850	25.	418	1.00	46.50	6
	ATOM	1249	CD1	LEU :	B 4	121	-2	0.529	69	.890	24.	255	1.00	45.15	6
20	ATOM	1250	CD2	LEU :	B 4	121	-2	1.383	70	.538	26.	486	1.00	51.31	6
	ATOM	1251	С	LEU :	B 4	121	-1	7.547	72	.452	24.	823	1.00	39.59	6
	ATOM	1252	0	LEU :	B 4	121	-1	7.975	73	.035	23.	836	1.00	40.66	8
	ATOM	1253	N	LEU :	B 4	122	-1	6.847	73	.059	25.	780	1.00	39.57	7
	MOTA	1254	CA	LEU :	B 4	122	-1	6.534	74	.478	25.	715	1.00	38.63	6
25	MOTA	1255	CB	LEU :	B 4	122	-1	5.829	74	.936	26.	992	1.00	41.79	6
	MOTA	1256	CG	LEU :		122		6.714	75	.149	28.	191	1.00	42.74	6
	MOTA	1257	CD1	LEU :		122	-1	5.911	75	.685	29.	360	1.00	42.89	6
	ATOM	1258	CD2	LEU		122		7.783		.162	27.	813	1.00	39.27	· 6
	MOTA	1259	С	LEU		122		5.677		.788	24.	513	1.00	40.47	6
30	ATOM	1260	0	LEU		122		5.823	75	.846		917		47.83	8
	MOTA	1261	N	MET		123		4.789		.853		. 168	1.00	34.27	7
	MOTA	1262	CA	MET		123		3.907		.019		024		35.25	6
	ATOM	1263	CB	MET		123		2.920		.858		922		32.56	6
25	MOTA	1264	CG	MET		123		2.013		.703		.125	1.00		6
35	ATOM	1265	SD	MET		123		0.345		.007		784	1.00		16
	MOTA	1266	CE	MET		423		0.770		.538		761	1.00		6
	MOTA	1267	С	MET		423		4.709		.100		.738		35.13	6
	ATOM	1268	0			423		4.341		.807		803		29.85	8
40	ATOM	1269	N			124		5.811		.361		704	1.00		7
40	ATOM	1270	CA	LYS		124		6.676		.354		544		32.29	6
	MOTA MOTA	1271 1272	CB	LYS				7.783		.316		736		30.56	6
	ATOM	1272	CG CD	LYS LYS				7.257		.879		843		30.07	6
	ATOM	1273	CE					6.444		.510		611		33.22	6
45	ATOM	1275	NZ	LYS				5.795		.136		706		28.75	6
73	ATOM	1276	C	LYS LYS				4.655		.067		678		31.01	7
	ATOM	1277	0	LYS				7.248		.754		304		29.26	6
	ATOM	1278	N	VAL				7.439		.149		166		30.22	8
	ATOM	1279	CA	VAL				7.495		.499		385		23.53	7
50	ATOM	1280	CB	VAL				8.278		150		278		28.91	6
50	ATOM	1280		VAL						.458		663		29.44	6
	ATOM	1282		VAL				8.633		.915		547		28.81	6
	ATOM	1282	C	VAL				9.401		733		354		31.22	6
	ATOM	1283	0	VAL				7.001		.682		498		32.03	6
55	ATOM	1285	Ŋ	THR				7.368		.465		629		31.95	8
55	ATOM	1286	CA	THR				5.721		.508		827		33.61	7
	ATOM	1287	CB	THR				4.645 3.270		.221		137		30.76	6
	ATOM	1288	OG1					3.270		.912		761		32.34	6
	111 011	1400	001	THE.	٠ ٦	U	12		10	.697	41.	941	1.00	33.07	8
							1.2	·							

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_	a mov	1289	CG2 T	HR B 4	26	-12.153	78.174	19.782	1.00 25		6
5 ,	ATOM	1299			26	-14.677	77.742	18.706	1.00 32		6
	MOTA	1291		HR B 4		-14.639	78.530	17.763	1.00 35		8
	MOTA	1292		SP B 4		-14.749	76.425	18.566	1.00 28		7
	MOTA				27	-14.796	75.807	17.257	1.00 3	5.12	6
	MOTA	1293		SPB4		-15.096	74.302	17.380	1.00 3	9.14	6
10	MOTA	1294		SP B 4		-13.910	73.496	17.806	1.00 4	5.80	6
	MOTA	1295				-12.786	73.774	17.348	1.00 4	1.97	8
	MOTA	1296		SP B 4	127	-14.064	72.517	18.583	1.00 5	0.06	8
	MOTA	1297	OD2 A			-15.883	76.502	16.429		3.94	6
	MOTA	1298			127	-15.673	76.815	15.262	1.00 3	8.02	8
15	MOTA	1299			127	-17.040	76.741	17.048	1.00 2		7
	MOTA	1300			428		77.388	16.367		9.99	6
	MOTA	1301	_		428	-18.154	77.190	17.168		2.49	6
	MOTA	1302			428	-19.448		17.089		25.54	6
	MOTA	1303			428	-20.086	75.818	18.012		20.60	6
20	MOTA	1304			428	-21.282	75.729	15.651	1.00 2		6
	MOTA	1305			428	-20.509	75.564			28.94	6
	ATOM	1306			428	-17.901	78.863	16.103		31.26	8
	ATOM	1307			428	-18.328	79.388	15.076		27.64	7
	MOTA	1308			429	-17.213	79.524	17.035		28.13	6
25	ATOM	1309		-	429	-16.894	80.937	16.883		29.59	6
	MOTA	1310	CB		429	-16.274	81.507	18.160		29.39 34.85	6
	ATOM	1311			429	-17.246	81.752				6
	MOTA	1312	CD	ARG B	429	-16.626	82.653			47.18	7
	MOTA	1313	NE	ARG B	429	-17.373				57.93	6
30	MOTA	1314	CZ	ARG B	429	-18.632				63.62	7
2.0	MOTA	1315	NH1	ARG B	429	-19.263				60.71	7
	ATOM	1316	NH2	ARG B	429	-19.238				62.38	6
	ATOM	1317		ARG B	429	-15.930				29.81	8
	ATOM	1318		ARG B	429	-16.101				30.81	7
35	MOTA	1319		MET B	430	-14.908				29.64	6
32	ATOM	1320		MET B	430	-13.920				34.72	6
	ATOM	1321		MET B	430	-12.939				34.97	
	ATOM	1322		MET B	430	-11.787				45.34	6
	MOTA	1323		MET B	430	-10.729	80.768			52.55	16
40		1324		MET B	430	-10.070				55.56	6
10	ATOM	1325		MET B		-14.638				34.01	6
	MOTA	1326		MET B	430	-14.39				37.29	8
	MOTA	132		ILE B	431	-15.51				29.99	7
	MOTA	1328		ILE E	431	-16.29				28.82	6
45				ILE E	3 431	-17.39				27.39	6
1.2	MOTA			ILE E	3 431	-18.31				23.87	6
	ATOM					-16.78	4 76.55			25.56	6
	ATOM					-17.82				17.29	6
	ATOM			ILE E		-16.95	3 80.28			29.49	6
50					3 431	-16.83	7 80.72	5 10.39		24.19	8
)(MOTA U				B 432	-17.65		4 12.47		25.25	7
					в 432	-18.35		2 12.17		30.38	6
	ATOM				B 432	-17.39		9 11.72		32.75	6
	ATOM				B 432	-17.53				36.38	8
_	ATOM				B 433	-16.43				26.77	7
5					B 433	-15.40				26.48	
	MOTA				B 433	-14.24				19.90	
	OTA				B 433	-14.90				30.73	6
	OTA	νı 124	:	UNIT							
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SUBSTITUTE SHEET (RULE 26)

5	7 TOM	1242	^	71 T T	_	422	14 040	05 100			
5	ATOM ATOM	1343	0	ALA			-14.849	85.432	10.171	1.00 31.60	8
		1344	N	CYS		434	-14.534	83.246	10.439	1.00 33.22	7
	ATOM	1345	CA	CYS		434	-14.023	83.021	9.120	1.00 34.34	6
	ATOM	1346	CB	CYS		434	-13.553	81.661	9.226	1.00 35.20	6
10	ATOM	1347	SG	CYS		434	-12.412	81.249	8.444	1.00 54.48	16
10	ATOM	1348	С	CYS		434	-15.106	83.116	8.062	1.00 34.09	6
	ATOM	1349	0	CYS		434	-14.844	83.555	6.952	1.00 34.89	8
	ATOM	1350	N	HIS	В	435	-16.318	82.699	8.394	1.00 34.30	7
	MOTA	1351	CA		В	435	-17.395	82.762	7.443	1.00 35.44	6
1.5	MOTA	1352	CB	HIS		435	-18.700	82.404	8.103	1.00 31.76	6
15	ATOM	1353	CG	HIS		435	-19.845	82.425	7.149	1.00 32.03	6
	MOTA	1354		HIS		435	-20.483	81.419	6.515	1.00 28.61	6
	MOTA	1355		HIS		435	-20.345	83.600	6.607	1.00 28.48	7
	MOTA	1356	CE1	HIS		435	-21.241	83.293	5.672	1.00 33.27	6
	ATOM	1357	NE2		В	435	-21.341	81.977	5.605	1.00 31.57	7
20	MOTA	1358	С	HIS		435	-17.528	84.152	6.878	1.00 32.74	6
	MOTA	1359	0	HIS		435	-17.842	84.326	5.715	1.00 32.87	8
	MOTA	1360	N	ALA		436	-17.315	85.121	7.758	1.00 31.01	7
	ATOM	1361	CA	ALA		436	-17.376	86.520	7.405	1.00 29.91	6
	MOTA	1362	CB	ALA	В	436	-17.008	87.352	8.618	1.00 21.23	6
25	MOTA	1363	С	ALA		436	-16.393	86.782	6.266	1.00 33.86	6
	MOTA	1364	0	ALA	В	436	-16.734	87.398	5.257	1.00 36.10	8
	MOTA	1365	N			437	-15.162	86.307	6.448	1.00 35.19	7
	MOTA	1366	CA	SER		437	-14.122	86.484	5.445	1.00 33.03	6
	ATOM	1367	CB	SER	В	437	-12.882	85.688	5.847	1.00 35.31	6
30	MOTA	1368	OG	SER		437	-11.855	85.824	4.879	1.00 44.99	8
	MOTA	1369	С	SER	В	437	-14.642	85.993	4.108	1.00 38.39	6
	MOTA	1370	0	SER	В	437	-14.700	86.730	3.127	1.00 37.54	8
	MOTA	1371	N	ARG	В	438	-15.008	84.719	4.096	1.00 37.32	7
	MOTA	1372	CA	ARG		438	-15.526	84.068	2.908	1.00 39.30	6
35	ATOM	1373	CB	ARG		438	-16.019	82.660	3.259	1.00 42.97	6
	ATOM	1374	CG	ARG		438	-14.910	81.673	3.590	1.00 41.72	6
	ATOM	1375	CĐ	ARG		438	-14.044	81.488	2.356	1.00 45.23	6
	MOTA	1376	NE	ARG		438	-14.781	80.936	1.235	1.00 45.66	7
4.0	MOTA	1377	CZ	ARG		438	-14.482	81.175	-0.040	1.00 49.71	6
40	MOTA	1378		ARG		438	-13.458	81.977	-0.347	1.00 50.91	7
	ATOM	1379		ARG			-15.219	80.619	-1.002	1.00 46.86	7
	MOTA	1380	С	ARG			-16.659	84.859	2.287	1.00 42.37	6
	ATOM	1381	0	ARG			-16.841	84.832	1.072	1.00 40.58	8
4 ~	ATOM	1382	N	PHE			-17.417	85.575	3.117	1.00 42.25	7
45	MOTA	1383	CA	PHE			-18.531	86.354	2.614	1.00 42.81	6
	MOTA	1384	CB	PHE			-19.198	87.132	3.731	1.00 42.18	6
	MOTA	1385	CG	PHE			-20.487	87.769	3.323	1.00 42.48	6
	MOTA	1386		PHE			-21.535	86.981	2.912	1.00 47.09	6
	MOTA	1387		PHE			-20.638	89.141	3.334	1.00 39.76	6
50	ATOM	1388		PHE			-22.735	87.543	2.527	1.00 49.17	6
	MOTA	1389	CE2	PHE			-21.851	89.717	2.944	1.00 45.10	6
	ATOM	1390	CZ	PHE	В	439	-22.901	88.911	2.538	1.00 46.36	6
	ATOM	1391	С	PHE	В	439	-18.016	87.319	1.581	1.00 44.79	6
	MOTA	1392	0	PHE	В	439	-18.514	87.354	0.465	1.00 40.26	8
55	ATOM	1393	N	LEU	В	440	-17.021	88.117	1.987	1.00 42.77	7
	ATOM	1394	CA	LEU	В	440	-16.415	89.115	1.109	1.00 42.96	6
	ATOM	1395	CB	LEU			-15.169	89.718	1.768	1.00 37.19	6
	ATOM	1396	CG	LEU	В	440	-15.477	90.588	2.967	1.00 36.97	6
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					010	OI PERME	4624 1	00 33.65	6
5	MOTA	1397	CD1 LEG	J B 440	-14.219	91.591	2.574 1.	00 35.42	6
,	ATOM	1398	CD2 LEG	J B 440	-16.577			00 45.47	6
	MOTA	1399	C LE	J B 440	-16.099	88.561		.00 52.48	8
	MOTA	1400	O LE	U B 440	-16.631	89.059		.00 49.15	7
	MOTA	1401		S B 441	-15.238	87.549	•	.00 54.76	6
10	ATOM	1402		S B 441	-14.929	86.956	- · -	.00 56.68	6
10		1403		S B 441	-14.150	85.700		.00 62.73	6
	ATOM	1404	CG HI		-12.713	85.934	- -	.00 65.73	6
	ATOM	1405	CD2 HI		-11.602	85.418	_ :		7
	MOTA	1405	ND1 HI	· 	-12.245	86.850	•	.00 66.01	6
	MOTA		CE1 H	-	-10.916	86.847	•	.00 65.55	7
15	MOTA	1407		S B 441	-10.512	85.993		.00 60.09	
	MOTA	1408		IS B 441	-16.217	86.633	- :	00 55.93	6
	MOTA	1409	_	IS B 441	-16.418	86.938		00 57.33	8
	MOTA	1410			-17.106	85.997		1.00 57.81	7
	MOTA	1411	_		-18.399	85.652		1.00 59.11	6
20	MOTA	1412	- -		-19.340	85.162		1.00 55.93	6
	MOTA	1413			-18.991	83.796		1.00 58.52	6
	MOTA	1414		ET B 442 ET B 442	-20.310	82.994		1.00 60.99	16
	MOTA	1415			-20.525	84.203		1.00 52.61	6
	MOTA	1416		ET B 442	-18.991		-2.785	1.00 60.31	6
25	MOTA	141		MET B 442	-19.646			1.00 58.18	8
	MOTA	141	_	MET B 442	-18.731			1.00 61.45	7
	MOTA	141	_	YS B 443	-19.267			1.00 64.90	6
	ATOM	142	•	LYS B 443	-19.182	_		1.00 64.40	6
	MOTA		_	LYS B 443	-20.160			1.00 69.12	6
30	MOTA		_	LYS B 443	-19.763			1.00 71.14	6
	MOTA			LYS B 443	-20.50			1.00 73.43	6
	ATOM			LYS B 443	-20.17			1.00 67.97	7
	ATOM		-	LYS B 443	-18.52			1.00 67.29	6
	ATOM			LYS B 443	-18.97			1.00 67.90	8
35	5 ATOM			LYS B 443	-17.38	-		1.00 66.57	7
	MOTA			VAL B 444	-16.58			1.00 64.76	
	MOTA			VAL B 444	-15.09	-		1.00 62.76	6
	OTA			VAL B 444	-14.26			1.00 64.00	6
	IOTA	M 14	31 CG1	VAL B 444	-14.20	_		1.00 59.27	6
4	O ATO			VAL B 444	-16.80			1.00 68.61	. 6
	ATO	M 14	33 C	VAL B 444	-16.96			1.00 70.60	8
	OTA	M 14	34 0	VAL B 444	-16.83			1.00 70.71	. 7
	ATO		35 N	GLU B 445	-16.9			1.00 71.45	5 6
	ATO		36 CA	GLU B 445	-16.1			1.00 72.36	
4	15 ATO		137 CB	GLU B 445	-14.7			1.00 40.00	
	ATC	_	138 CG	GLU B 445	-13.9			1.00 40.00	
	ATC	-	139 CD	GLU B 445	-14.5			1.00 40.00	
	ATC	OM 14	440 OE1		-14.3		_	1.00 40.0	0 8
	OTA	1°	441 OE2		-12.7		- -	1.00 71.4	6 6
	50 ATC	~ 1	442 C	GLU B 445	-18.6	_			2 8
	ATO	OM 1	443 0	GLU B 445					
	ATO		444 N	CYS B 446			= :		
	AT		445 CA	CYS B 446					5 6
	AT		446 CB	CYS B 446					3 16
	55 AT		447 SG	CYS B 446					1 6
			448 C	CYS B 446					6 8
			449 0	CYS B 446		_			2 7
			450 N	PRO B 447		220 86.3	220 -0.23		
					123				

5	ATCM	1451	CD	PRO 1	B 447	-22.837	85.637	-8.886	3 00	72 00	_
	ATOM	1452	CA	PRO 1		-23.461	87.997			72.88	6
	ATOM	1453	СВ	PRO 1		-24.399	87.338	-9.659		74.22	6
	MOTA	1454	CG	PRO 1		-23.981	85.934	-9.039 -9.776		72.98	6
	ATOM	1455	С	PRO 1		-24.203	88.519	-7.451		74.77	6
10	ATOM	1456	0	PRO 1		-24.601	87.749			75.94	6
	ATOM	1457	N	THR		-24.390		-6.611		76.67	8
	ATOM	1458	CA	THR		-25.134	89.828	-7.373		76.91	7
	ATOM	1459	СВ	THR I			90.436	-6.268		78.24	6
	ATOM	1460	0G1			-24.883	91.948	-6.276		81.33	6
15	MOTA	1461	CG2			-25.474	92.525	-7.451		84.46	8
	ATOM	1462	C	THR		-23.394	92.234	-6.269		83.51	6
	ATOM	1463	Ö	THR I		-26.594	90.160	-6.619		77.42	6
	ATOM	1464	N	GLU I		-27.512	90.649	-5.982		77.65	8
	ATOM	1465	CA	GLU I		-26.759	89.400	-7.697		76.29	7
20	ATOM	1466	CB	GLU I		-28.051	.89.017	-8.211		75.03	6
	ATOM	1467	CG	GLU E		-27.923	88.915	-9.719		74.62	6
	ATOM	1468	CD	GLU E		-28.823		-10.343		40.00	6
	ATOM	1469	OE1			-28.522		-11.756	1.00	40.00	6
	ATOM	1470	OE2			-27.366		-12.190	1.00	40.00	8
25	ATOM	1471	C	GLU E		-29.449		-12.492	1.00	40.00	8
20	ATOM	1472	0			-28.448	87.660	-7.609	1.00	73.49	6
	ATOM	1472	N	GLU E		-29.479	87.092	-7.953	1.00	70.24	8
	ATOM	1474		LEU E		-27.624	87.158	-6.695	1.00		7
	ATOM	1475	CA CB	LEU E		-27.879	85.879	-6.058	1.00	68.82	6
30	ATOM	1476	CG	LEU E		-26.772	84.887	-6.447	1.00	71.91	6
50	ATOM	1477	CD1	LEU E		-26.612	84.503	-7.900	1.00	76.62	6
	ATOM	1478	CD1			-25.396	83.637	-8.059	1.00	77.95	6
	ATOM	1479	C D Z			-27.849	83.775	-8.351	1.00	76.46	6
	ATOM	1480	0	LEU E		-27.941	86.012	-4.536		56.22	6
35	ATOM	1481	N	PHE B		-28.251	85.039	-3.849		56.01	8
	ATOM	1482	CA	PHE B		-27.666	87.215	-4.012		51.96	7
	ATOM	1483	CB	PHE B		-27.635	87.494	-2.585	1.00 5	8.44	6
	ATOM	1484	CG	PHE B		-26.579	88.573	-2.263		51.34	6
	ATOM	1485	CD1	PHE B		-25.153	88.078	-2.413		3.02	6
40	ATOM	1486	CD2	PHE B		-24.675	87.587	-3.626	1.00 6		6
	MOTA	1487		PHE B		-24.283	88.173	-1.346	1.00 6		6
	ATOM	1488		PHE B		-23.327	87.217	-3.757	1.00 6		6
	ATOM	1489	CZ	PHE B		-22.939	87.806	-1.472	1.00 6		6
	ATOM	1490	C	PHE B		-22.459	87.335	-2.686	1.00 6		6
45	ATOM	1491	0	PHE B		-28.931	87.994	-1.962	1.00 5		6
	ATOM	1492	N	PRO B		-29.207	89.214	-1.908	1.00 5		8
	ATOM	1493	CD			-29.791	87.072	-1.473	1.00 5		7
	ATOM	1494	CA	PRO B		-29.767	85.611	-1.494	1.00 5		6
	ATOM	1495		PRO B		-31.037	87.598	-0.843	1.00 5	0.26	6
50	ATOM	1496	CB	PRO B		-31.746	86.375	-0.301	1.00 4	9.19	6
50	ATOM		CG	PRO B		-31.024	85.197	-0.842	1.00 4	5.89	6
	ATOM	1497	C	PRO B		-30.636	88.567	0.251	1.00 4	9.62	6
	ATOM	1498	0	PRO B		-29.628	88.401	0.906	1.00 5	2.35	8
		1499	N	PRO B		-31.494	89.539	0.535	1.00 5	1.50	7
55	ATOM	1500	CD	PRO B		-32.853	89.644	0.022	1.00 4		6
,,	ATOM	1501	CA	PRO B		-31.184	90.573	1.530	1.00 5		6
	ATOM	1502	CB	PRO B		-32.422	91.401	1.625	1.00 5		6
	ATOM	1503	CG	PRO B		-33.378	90.827	0.724	1.00 50		6
	ATOM	1504	С	PRO B	453	-30.829	90.039	2.906	1.00 50		6
						124					-

	W O 33	700014							
_			0 DD	O B 453	-29.700	90.206			3
5	ATOM	1505	_		-31.807		3.631 1	•	7
	MOTA	1506		-	-31.538	-	4.948 1	.00 47.17	6
	MOTA	1507		U B 454	-32.550	87.858		.00 44.44	6
	MOTA	1508		U B 454		87.412		.00 41.33	6
	MOTA	1509		U B 454	-32.347				6
10	MOTA	1510	CD1 LE	U B 454	-31.987	88.589		1.00 34.79	6
10	ATOM	1511	CD2 LE		-33.590	86.732			6
		1512		EU B 454	-30.099	88.443		1.00 42.25	
	MOTA		-	EU B 454	-29.323	88.774		1.00 40.82	8
	MOTA	1513	-	HE B 455	-29.716	87.707		1.00 39.29	7
	MOTA	1514			-28.347	87.204	3.770	1.00 41.81	6
15	MOTA	1515			-28.132	86.536	2.418	1.00 47.22	6
	MOTA	1516		HE B 455		85.836	2.292	1.00 56.97	6
	MOTA	1517	_	HE B 455	-26.813	84.915	3.247	1.00 57.23	6
	MOTA	1518	CD1 P	HE B 455	-26.437		1.236	1.00 59.40	6
	MOTA	1519	CD2 P	HE B 455	-25.949	86.094		1.00 56.58	6
20	ATOM	1520	CE1 P	HE B 455	-25.225	84.234	3.153		6
20	ATOM	1521		HE B 455	-24.720	85.409	1.134		
		1522		HE B 455	-24.360	84.481	2.103	1.00 59.94	6
	MOTA			HE B 455	-27.400	88.386	3.923	1.00 45.12	6
	MOTA	1523	-	PHE B 455	-26.657	88.450	4.889	1.00 39.95	8
	MOTA	1524		LEU B 456	-27.439	89.303	2.949	1.00 43.92	7
25	MOTA	1525			-26.597		2.947	1.00 44.08	6
	ATOM	1526		LEU B 456	-27.001		1.802	1.00 50.20	6
	MOTA	1527	-	LEU B 456			0.432	1.00 55.79	6
	MOTA	1528	-	LEU B 456	-26.439		-0.591	1.00 54.70	6
	MOTA	1529		LEU B 456	-27.064		0.494	1.00 53.01	6
30	ATOM	1530		LEU B 456	-24.920			1.00 44.65	6
50	ATOM	153		LEU B 456	-26.689		4.264	1.00 45.93	8
	ATOM	153		LEU B 456	-25.678		4.886		7
	MOTA	153		GLU B 457	-27.990		4.265		6
		153	-	GLU B 457	-28.288	92.016	5.497	1.00 46.37	
2.5	ATOM		_	GLU B 457	-27.434	91.452	6.628	1.00 43.60	6
35				GLU B 457	-26.75		7.339	1.00 42.69	8
	MOTA			GLU B 457	-29.76		5.855	1.00 50.16	6
	ATOM			GLU B 457	-30.20		6.954	1.00 20.00	6
	ATOM			GLU B 457	-31.64		6.782	1.00 20.00	6
	MOTA				-32.35		5.779	1.00 20.00	8
4() ATOM			GLU B 457	-32.15		7.638	1.00 20.00	8
	MOTA			GLU B 457	-27.42		7.281	1.00 43.21	7
	MOTA			VAL B 458	-26.70		8.351	1.00 44.98	6
	OTA	1 154		VAL B 458			8.432		6
	OTA	4 15	44 CB	VAL B 458	-27.07		9.646		6
4	5 ATO	<u>4</u> 15		VAL B 458	-26.44				6
•	OTA	_	46 CG2	VAL B 458	-28.56				6
	ATO			VAL B 458	-25.19		_		8
	ATO			VAL B 458	-24.55				7
				PHE B 459	-24.60				
_	ATO		50 CA	PHE B 459	-23.16	65 89.480	7.077	1.00 48.18	6
5	OTA 0			PHE B 459	-22.74		6.065	1.00 43.60	6
	OTA		51 CB		-23.1			1.00 40.79	6
	OTA		52 CG		-24.4			3 1.00 41.01	6
	OTA			PHE B 459	-24.4				6
	ATC			2 PHE B 459					
4	55 ATC		555 CE		-24.8				
•	ATC		556 CE		-22.6	49 85.09			
	ATO		557 CZ	PHE B 459	-23.9				
	ATO		558 C	PHE B 459	-22.6	27 90.75	6.62	3 1.00 52.71	. 0
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5	71 671 (1550	_	PHE	ъ	450	21 414	01 050	C 701	1 00 51 24	•
3	ATOM.	1559	0				-21.414	91.050	6.791	1.00 51.34	8
	MOTA	1560	N	GLU		460	-23.489	91.531	5.976	1.00 62.92	7
	MOTA	1561	CA	GLU		460	-22.953	92.741	5.533	1.00 69.33	6
	ATOM	1562	CB	GLU		460	-23.851	93.487	4.505	1.00 72.95	6
10	MOTA	1563	CG	GLU		460	-22.917	94.002	3.412	1.00 78.35	6
10	MOTA	1564	CD	GLU		460	-22.908	95.480	3.256	1.00 82.97	6
	MOTA	1565	OE1	GLU		460	-23.257	96.213	4.217	1.00 88.28	8
	MOTA	1566	OE2	GLU		460	-22.524	95.977	2.167	1.00 84.80	8
	MOTA	1567	С	GLU	В	460	-22.790	93.576	6.786	1.00 71.87	6
	MOTA	1568	0	GLU	В	460	-23.471	93.391	7.802	1.00 74.51	8
15	MOTA	1569	N	ASP	В	461	-21.796	94.449	6.696	1.00 78.50	7
	MOTA	1570	CA	ASP	В	461	-21.401	95.328	7.701	1.00 84.19	6
	MOTA	1571	CB	ASP	В	461	-20.182	96.032	7.125	1.00 85.82	6
	ATOM	1572	CG	ASP	В	461	-19.261	95.066	6.463	1.00 89.62	6
	ATOM	1573	OD1	ASP		461	-19.670	93.929	5.982	1.00 93.00	8
20	ATOM	1574		ASP		461	-18.084	95.361	6.387	1.00 93.04	8
	ATOM	1575	С	ASP		461	-22.540	96.291	8.012	1.00 86.80	6
	ATOM	1576	Ō	ASP		461	-23.063	96.176	9.139	1.00 88.70	8
	ATOM	1577	OXT	ASP		461	-22.962	97.048	7.098	1.00 88.70	8
	TER		01.1		_		22.502	37.040	7.050	1.00 00.70	U
25	ATOM	4002	C1	Т3	J	1	20.152	36.643	29.561	1.00 22.34	6
	ATOM	4003	C2	T3	J	î	19.021	41.567	29.283	1.00 22.34	6
	ATOM	4004	C3	T3	J	1	18.880	37.086	29.226	1.00 21.84	6
	ATOM	4005	C4	T3	J	1	18.249	42.606	28.776	1.00 23.43	
	ATOM	4006	C5	T3	J	1	18.747	38.372	28.866		6
30	ATOM	4000	C6	T3	J	1	17.938			1.00 24.83	6
30	ATOM	4007	C7	T3	J			43.621	29.664	1.00 25.16	6
	ATOM	4008	C8	T3	J	1	19.799	39.296	28.753	1.00 24.65	6
	ATOM	4009	C9.	13 T3	J	1	18.330	43.594	31.028	1.00 21.93	6
	ATOM	4010		T3	J	1	21.101	38.940	29.075	1.00 25.09	6
35			C10 C11			1	19.063	42.558	31.465	1.00 23.66	6
33	ATOM	4012 4013	C11	T3	J	1	21.254	37.600	29.456	1.00 23.12	6
	ATOM	4013	C12	Т3	J	1	19.459	41.490	30.621	1.00 19.67	6
	ATOM	4014		Т3	J	1	20.370	35.228	30.075	1.00 18.97	6
	ATOM		C15		J	1	21.549	34.480	29.455	1.00 19.32	6
40	ATOM	4016	C17	T3	J	1	21.535	33.003	29.710	1.00 19.02	6
40	ATOM	4017	I1	Т3	J	1	16.898	39.029	28.661	1.00 25.29	53
	ATOM	4018	12	Т3	J	1	17.058	45.327	29.154	1.00 26.49	53
	ATOM	4019	13	T3	J	1	22.763	40.262	29.169	1.00 25.67	53
	ATOM	4020	N1	T3	J	1	21.800	34.859	28.024	1.00 15.12	7
4.5	MOTA	4021	01	T3	J	1	17.934	44.682	31.806	1.00 21.79	8
45	MOTA	4022	02	T3	J	1	19.432	40.560	28.362	1.00 22.05	8
	MOTA	4023	03	Т3	J	1	21.911	32.260	28.776	1.00 20.38	8
	MOTA	4024	04	ТЗ	J	1	21.137	32.622	30.840	1.00 20.16	8
	TER										
	ATOM	4025	C1	Т3	K,		-28.131	75.928	7.543	1.00 22.34	6
50	ATOM	4026	C2	T 3	K		-24.676	77.673	4.318	1.00 21.84	6
	MOTA	4027	C3	Т3	K		-28.490	76.351	6.201	1.00 23.43	6
	ATOM	4028	C4	Т3	K	1	-24.217	77.893	2.989	1.00 22.31	6
	ATOM	4029	C5	TЗ	K		-27.485	76.499	5.233	1.00 24.83	6
	ATOM	4030	C6	TЗ	K	1	-23.545	79.124	2.700	1.00 25.16	6
55	ATOM	4031	C7	Т3	K	1	-26.132	76.227	5.581	1.00 24.65	6
	MOTA	4032	C8	Т3	K	1	-23.382	80.104	3.772	1.00 21.93	6
	MOTA	4033	C9	Т3	K	1	-25.685	75.833	6.855	1.00 25.09	6
	ATOM	4034	C10	тЗ	K	1	-23.867	79.823	5.042	1.00 23.66	6
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SUBSTITUTE SHEET (RULE 26)

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			011	m S	K	1	-26.70	8	75.	570	7.83		.00			6	
5	MOTA	4035	C11	T3	K	1	-24.52		78.	610	5.37		1.00			6	
	MOTA	4036	C12		K	1	-29.21		75.		8.62		1.00			6	
	ATOM	4037	C13		K	1	-29.18		74.		9.4		1.00			6	
	MOTA	4038	C15			1	-30.4		74.		10.2		1.00			6	
	MOTA	4039	C17	T3	K		-27.80			342	3.3	16	1.00			53	
10	MOTA	4040	I1	T3	K	1	-22.7			619	0.8		1.00	26	.49	53	
	MOTA	4041	12	T3	K	1	-23.6			792	7.3		1.00	25	. 67	53	
	MOTA	4042	13	Т3	K	1	-23.6	0 A		342	8.7		1.00			7	
	MOTA	4043	Nl	Т3	K	1	-28.6			265	3.4		1.00			8	
	MOTA	4044	01	т3	K	1	-22.7			388	4.5		1.00			8	
15	MOTA	4045	02	т3	K	1	-25.2			.159	10.3		1.00			8	
	MOTA	4046	03	Т3	K	1	-30.8				10.7		1.00			8	
	MOTA	4047	04	Т3	K	1	-31.0	28	15	.359	10.	123	1.0	,			
	TER									176	48.8	000	1.00	0 40	0.00	6	
	ATOM	1	С		s x		13.8			.176					0.00	8	
20	ATOM	2	0			686	13.9			.120	47.				0.00	7	
20	ATOM	3		LY	s x	686	14.3			.245	50.				0.00	6	
	MOTA	4				686	14.9			.070	49.				0.00	7	
	MOTA	5				687	13.			.527	49.					6	
,		6				687	11.			.518		521			0.00	6	
		7				687	10.			000.		212			0.00	6	
25	MOTA	8				687	10.	981		.526		563			0.00		
	MOTA	9	-			687	11.	021	38	3.908		753			0.00	7	
	MOTA	10)1 H	ts X	687	11.	354		0.844		754			0.00		
	MOTA	1:				687		614	4(0.994		.034			0.00	6	
20	MOTA	1:				687	11.	422	3	9.847		646			0.00		7
30	MOTA	1:		12 11 H	TS X	687		183		8.108		.208			0.00		5
	MOTA	1	_			687	11.	674		8.361		.094			0.00		3
	MOTA	1				ζ 688		064		7.458		.649			10.00		7
	MOTA		_			₹ 688		911		6.858		.931	1.	-	10.00		6
	MOTA	1	7 C			k 688		.292		7.850		.968			10.00		6
35			8 C			x 688	9	.246	5 3	5.573	-	.161			40.00		6
	MOTA					x 688		.319		4.473		.722			40.00		8
	ATOM	_				x 689		.42		5.75		.865			40.00		7
	ATOM					x 689		.66		34.64	0 44	.924			40.00		6
	ATOM					x 689		.73	_	35.16	7 43	.498			40.00		6
4(x 689		.63		34.05	3 42	2.453			40.00		6
	MOTA					x 689		.59		36.14		3.176			40.00		6
	MOTA			701	11 E	x 689		.25		36.18		1.688			40.0		6
	MOTA				TIE	x 689		.95		33.86	9 45	5.228			40.0		6
	1OTA					x 689		.92		32.65	7 45	5.51			40.0		8
4						x 690		2.06		34.57		5.140			40.0		7
	IOTA					x 690		3.39		33.99	6 4	5.39	7 1	.00	40.0	0	6
	ATO		_			x 690		1.34		35.04		5.89			40.0		6
	OTA					x 690		4.45		36.16	58 4	4.90			40.0		6
	ATO!		-					5.39		37.26		5.36			40.0		6
5	OTA 0					X 690		4.94		35.69		3.54	0 1		40.0		6
	OTA	M			PEO	x 690		3.2		32.99		6.46			40.0		6
	OTA			С		X 690		3.6		31.83		6.31	5 1		40.0		8
	ATO		35	0		X 690		2.7		33.4		7.54	1 1		40.0		7
	ATC	M	36	N		X 691		2.5		32.5		8.56			40.0		6
:	55 ATC	MC	37	CA		x 691		1.7		33.2		9.65	-		40.0		6
	ATC	MC	38	CB		X 691		2.5		34.1		50.56			40.0		6
	ATO	MC	39	CG		X 691		3.6		33.8		51.38			40.0		6
	ATO	MC	40	CD2	HIS	x 691			40	55.0	<i></i>		-				
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									1 00 6	0 00	~
5	MOTA	41	ND1	HIS X	691	12.359	35.484	50.669	1.00 4		7
	MOTA	42	CEl	HIS X	691	13.242	35.991	51.513		0.00	6
	MOTA	43	NE2	HIS X	691	14.016	35.031	51.949		0.00	7
	MOTA	44	С	HIS X	691	11.954	31.331	47.861		0.00	6
	ATOM	45	0		691	12.505	30.240	47.882		0.00	8
10	ATOM	46	N	ARG X		10.839	31.494	47.167	1.00 4	0.00	7
10	ATOM	47	CA	ARG X		10.169	30.333	46.518	1.00 4	0.00	6
	ATOM	48	CB	ARG X		9.118	30.800	45.517	1.00 4	0.00	6
	ATOM	49	C	ARG X		11.153	29.402	45.752	1.00 4	0.00	6
		50	0	ARG X		11.030	28.168	45.779	1.00 4	0.00	8
1.5	ATOM				693	12.117	30.000	45.072		0.00	7
15	ATOM	51	N		693	13.078	29.252	44.226		10.00	6
	ATOM	52	CA		693	13.784	30.210	43.274		10.00	6
	MOTA	53	CB			12.796	31.012	42.432		10.00	6
	MOTA	54	CG		693		31.012	41.458		10.00	6
	ATOM	55	CD1		693	13.479		41.430		10.00	6
20	MOTA	56	CD2			11.884	30.126			40.00	6
	MOTA	57	С	LEU X		14.143	28.531	45.054		40.00	8
	MOTA	58	0	LEU X		14.702	27.508	44.633			7
	MOTA	59	N	LEU X		14.400	29.079	46.209		40.00	
	MOTA	60	CA	TEA >		15.407	28.538	47.115		40.00	6 6
25	MOTA	61	CB	LEU >		15.871	29.626	48.084		40.00	
	MOTA	62	CG	TEO >		16.692	30.716	47.404		40.00	6
	MOTA	63	CD1	LEU X	k 694	17.279	31.724	48.391		40.00	6
	ATOM	64	CD2	LEU X	x 694	17.879	30.156	46.619		40.00	6
	ATOM	65	С	LEU X	x 694	14.837	27.404	47.957		40.00	6
30	ATOM	66	0	LEU 3	X 694	15.555	26.747	48.716		40.00	8
	MOTA	67	N	GLN :	X 695	13.554	27.157	47.809		40.00	7
	MOTA	68	CA	GLN :	X 695	12.883	26.188	48.685		40.00	6
	MOTA	69	С	GLN :	X 695	12.423	24.910	47.977		40.00	6
	MOTA	70	0	GLN :	x 695	12.309	23.845	48.598		40.00	8
35	ATOM	71	СВ		X 695	11.681	26.858	49.322		40.00	6
55	ATOM	72	CG		X 695	12.074	28.125	50.080		20.00	6
	ATOM	73	CD		X 695	10.899	28.768	50.801		20.00	6
	ATOM	74	OE		X 695	9.772	28.296	50.671	1.00	20.00	8
	MOTA	75	NE		X 695	11.092	29.828	51.560	1.00	20.00	7
40	ATOM	76	N		X 696	12.155	25.020	46.714	1.00	40.00	7
70	ATOM	77			X 696	11.698	23.885	45.910	1.00	40.00	6
	MOTA	78			x 696	11.450		44.497	1.00	40.00	6
	ATOM	79			x 696	10.782			1.00	40.00	6
	ATOM	80		1 ASP		10.550			1.00	40.00	8
45	ATOM	81		2 ASP		10.449			1.00	40.00	8
43	MOTA	82			X 696	12.774				40.00	6
		83			X 696	13.937				40.00	8
	ATOM				X 697	12.370				40.00	7
	ATOM	84			X 697	13.258				40.00	6
	ATOM	85				12.685				40.00	6
50		86			X 697	12.535				40.00	8
	MOTA	87			X 697					40.00	6
	ATOM	88			X 697	13.329				40.00	8
	MOTA	89			X 697	14.24				40.00	7
	ATOM	90			X 698	12.35				40.00	6
55		91			X 698	11.98				40.00	6
	MOTA	92			X 698	11.693					8
	MOTA	93			X 698	10.51				40.00	6
	ATOM	94	4 C	SER	X 698	12.88	7 18.340	41.758	3 1.00	40.00	0
						128					

_						12.052	17 150	40.006	1 00 40 00	
5	ATOM	95		SER X		13.253	17.158 18.976	42.026 40.714	1.00 40.00	8 8
	MOTA	96	OXT	SER X	698	13.131	10.976	40.714	1.00 40.00	0
	TER	-	CD	TVC V	C00	-33.793	96.885	6.491	1.00 40.00	6
	MOTA	1		LYS Y	688	-35.793 -35.002	95.370	8.130	1.00 40.00	6
10	MOTA	2		LYS Y		-36.027	95.520	8.779	1.00 40.00	8
10	ATOM	3		LYS Y		-30.027	96.619	8.695	1.00 40.00	7
	MOTA	4			688 688	-34.040	96.591	7.954	1.00 40.00	6
	ATOM	5		LYS Y		-34.578	93.781	6.908	1.00 40.00	7
	ATOM	6		IPE A		-35.862	93.701	7.268	1.00 40.00	6
1.5	ATOM	7	CA CB		689	-35.971	91.759	6.572	1.00 40.00	6
15	MOTA	8 9	CG2	ILE Y	689	-37.270	91.077	6.932	1.00 40.00	6
	MOTA	10	CG2	ILE Y	689	-35.917	91.937	5.062	1.00 40.00	6
	MOTA	11	CD1	ILE Y	689	-36.341	90.691	4.289	1.00 40.00	6
	MOTA MOTA	12	CDI		689	-36.032	92.870	8.780	1.00 40.00	6
20	MOTA	13	0		689	-36.913	93.446	9.442	1.00 40.00	8
20	ATOM	14	N	LEU Y		-35.019	92.834	9.787	1.00 40.00	7
	ATOM	15	CA	LEU Y		-34.956	92.320	11.163	1.00 40.00	6
	ATOM	16	CB	LEU Y		-33.528	92.432	11.697	1.00 40.00	6
	ATOM	17	CG		690	-32.516	91.647	10.864	1.00 40.00	6
25	MOTA	18	CD1		690	-31.087	91.764	11.397	1.00 40.00	6
20	ATOM	19	CD2		690	-32.819	90.148	10.812	1.00 40.00	6
	ATOM	20	C		690	-35.899	93.123	12.065	1.00 40.00	6
	MOTA	21	Ō		690	-36.570	92.492	12.928	1.00 40.00	8
	MOTA	22	N		691	-36.039	94.731	11.373	1.00 40.00	7
30	MOTA	23	CA		691	-36.634	94.923	12.683	1.00 40.00	6
	MOTA	24	CB	HIS Y	691	-36.854	96.383	12.935	1.00 40.00	6
	ATOM	25	CG	HIS Y	691	-35.610	97.153	13.078	1.00 40.00	6
	MOTA	26	CD2	HIS Y	691	-34.757	97.640	12.159	1.00 40.00	6
	MOTA	27	ND1		691	-35.129	97.579	14.319	1.00 40.00	7
35	MOTA	28	CE1			-34.039	98.290	14.122	1.00 40.00	6
	MOTA	29	NE2			-33.786	98.346	12.815	1.00 40.00	7
	MOTA	30	С	HIS Y		-37.972	94.287	12.756	1.00 40.00	6
	MOTA	31	0	HIS Y		-38.240	93.417	13.545	1.00 40.00	8
	MOTA	32		ARG Y		-38.265	94.388	11.505	1.00 40.00	7
40	ATOM	33		ARG Y		-39.577	93.869	11.276	1.00 40.00	6
	MOTA	34		ARG Y		-39.653	93.692	9.795	1.00 40.00	6 6
	ATOM	35		ARG Y		-40.759	92.764	9.329 7.848	1.00 40.00 1.00 40.00	6
	MOTA	36		ARG Y		-40.618	92.422 92.641	7.040	1.00 40.00	7
15	ATOM	37		ARG Y		-41.849 -41.898	92.758	5.763	1.00 40.00	6
45	ATOM	38 39		ARG 3		-40.784	92.730	5.024	1.00 40.00	7
	ATOM	40		ARG :		-43.034	92.940	5.080	1.00 40.00	7
	ATOM	41		ARG Y		-39.941	92.547	11.995	1.00 40.00	6
	ATOM ATOM	42		ARG S		-41.001	92.440	12.649	1.00 40.00	8
50	ATOM	43		LEU :		-39.095	91.576	11.816		7
50	ATOM	44		LEU :		-39.230	90.232	12.395	1.00 40.00	6
	ATOM	45		LEU :		-38.362	89.337	11.615	1.00 40.00	6
	ATOM	46		LEU :		-38.737	89.375	10.132	1.00 40.00	6
	ATOM	47				-37.794	88.570	9.247		6
55	ATOM	48				-40.142		9.862		6
	ATOM	49			r 693	-38.921		13.816		6
	ATOM	50			Y 693	-39.191		14.615		8
	ATOM	51		LEU :	Y 694	-38.366	91.533	14.076	1.00 40.00	7
						129				

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5	MOTA	52	CA	LEU	Y	694	-38.174	91.885	15.435	1.00	40.00	6
	MOTA	53	CB	LEU	Y	694	-37.181	93.002	15.561	1.00	40.00	6
	ATOM	54	CG	LEU	Y	694	-35.799	92.377	15.869	1.00	40.00	6
	MOTA	55	CD1	LEU	Y	694	-34.897	93.275	16.702	1.00	40.00	6
	ATOM	56	CD2	LEU	Y	694	-35.897	91.055	16.661	1.00	40.00	6
10	MOTA	57	С	LEU	Y	694	-39.596	91.903	15.915	1.00	40.00	6
	MOTA	58	0	LEU	Y	694	-39.985	91.253	16.858	1.00		8
	MOTA	59	N	GLN	Y	695	-40.787	92.229	15.048	1.00	40.00	7
	ATOM	60	CA	GLN	Y	695	-42.034	91.457	15.543	1.00	40.00	6
	ATOM	61	С	GLN	Y	695	-43.054	90.901	14.240	1.00	40.00	6
15	ATOM	62	0	GLN	Y	695	-43.102	91.557	13.189	1.00	40.00	8
	MOTA	63	CB	GLN	Y	695	-42.362	92.025	16.923	1.00	40.00	6
	ATOM	64	CG	GLN	Y	695	-41.013	92.101	17.768	1.00	40.00	6
	ATOM	65	CD	GLN	Y	695	-40.943	91.235	19.059	1.00	40.00	6
	MOTA	66	OE1	GLN	Y	695	-41.828	90.426	19.318	1.00	40.00	8
20	ATOM	67	NE2	GLN	Y	695	-39.938	91.399	19.916	1.00	40.00	7
	ATOM	68	N	ASP	Y	696	-43.802	89.498	14.402	1.00	40.00	7
	ATOM	69	CA	ASP	Y	696	-44.784	88.354	13.428	1.00	40.00	6
	ATOM	70	С	ASP	Y	696	-46.034	88.934	12.759	1.00	40.00	6
	ATOM	71	0	ASP	Y	696	-46.266	88.655	11.529	1.00	40.00	8
25	ATOM	72	CB	ASP	Y	696	-45.211	87.192	14.322	1.00	40.00	6
	MOTA	73	, CG	ASP	Y	696	-44.021	86.560	15.058	1.00	40.00	6
	ATOM	74	OD1	ASP	Y	696	-42.823	86.994	14.844	1.00	40.00	8
	MOTA	75	OD2	ASP	Y	696	-44.212	85.591	15.889	1.00	40.00	8
	END									,		
30												

5 Appendix 2

Atomic Coordinates for Human ERa Complexed with DES, and a GRIP1 NR-box 2 Peptide

	Atomic Coordinates for Human ERa Complexed with DES, and a Gittle 1112 5000 1													
	CRYST1	54.094			8.04			111.		90.00			L 2	
10				0.000	00	0.000	000	0.00	0000					•
	ORIGX1	1.000		L.0000	0 0 0 0	0.000			0000					
	ORIGX2	0.000	_	0.0000	00	1.000	000	0.00	0000					
	ORIGX3	0.00		0.0000	00	0.007		0.0	0000					
	SCALE1	0.01		0.0121		0.000			0000					
15	SCALE2	0.00		0.0000		0.018		0.0	0000					
	SCALE3	0.00	0000	0.0000		• • •								5 2 26
		_	CD	SER	A	305	35.			787 -1				73.26
	MOTA	-				305		331 -	-14.		L.289			72.95 72.46
	MOTA	2	-			305			-13.	-	1.186			74.06
20	MOTA	3	-	-	A	305	36		-16.		285		.00	73.59
	MOTA	4 5	CA	SER	A	305		.138	-14.		0.061		.00	72.21
	ATOM	5 6	N	LEU	A	306			-14.	-	2.449		.00 .00	71.05
	MOTA	7	CA	LEU	A	306			-13.		3.702		.00	70.19
25	MOTA	8	CB	LEU	A	306			-14.		4.878		.00	69.57
25	MOTA MOTA	9	C	LEU	Α	306			-12.		3.719		.00	69.96
	MOTA	10	0	LEU	A	306		.580	-11.		4.43		.00	68.06
	MOTA	11	N	ALA	A	307		.851		.176	4.54		.00	64.88
	MOTA	12	CA	ALA	Α	307 -		.358	-10	.810	4.43		00	65.83
30	MOTA	13	CB	ALA	A	307		841	-10	.795 .204	5.86		00	63.36
30	MOTA	14	С	ALA	A	307	33	.792	- TO	.984	6.00		00	62.73
	MOTA	15	0	ALA	A	307	33	3.878		.062	6.84		L.00	62.52
	MOTA	16	N	LEU	A	308		1.064		.598	8.15		1.00	62.57
	MOTA	17	CA	LEU	A	308		1.487 4.423		.745	9.17		1.00	62.81
35		18	CB	LEU	A	308		3.214		.688	9.13		1.00	64.21
	MOTA	19	CG	LEU	A	308		3.214		.513	10.40		1.00	66.28
	MOTA	20	CD1	LEU	A	308		1.919		898	8.98		1.00	63.80
	MOTA	21	CD2	LEU	A	308 308		5.903		0.037	8.1	00	1.00	
	MOTA	22	С	LEU	A.	308		6.385		9.445	9.0		1.00	_
40	MOTA (23	0	LEU	A A	309		6.561		0.219	6.9	-	1.00	_
	MOTA	24	N	SER	A A	309		7.928		9.743	6.7	_	1.00	
	MOTA	25	CA	SER SER	A	309		8.720) -1	0.750	5.9		1.00	
	MOTA	26	CB	SER	Ā	309		8.889	-1	0.283	4.6		1.00	
	MOTA	27	OG C	SER	A	309	3	37.986	-	8.373	6.0		1.00	
4:		28	C 0	SER		309	3	88.96		7.637	6.2		1.00	
	MOTA		N	LEU		310		36.940		8.038			1.00	
	ATOM		CA	LEU		310	:	36.87		6.759			1.00	
	ATOM		CB	LEU		310		35.51		6.596			1.00	
_	MOTA O		CG	LEU		310		35.30		7.188			1.00	
3	MOTA 0		CD1			310		33.95	_	6.728		055	1.0	
	MOTA MOTA		CD2			310		36.41		6.755		650	1.0	
	ATOM	_	C	LEU		310		37.08		-5.589		609 741	1.0	
	MOTA		Ö	LEU		310		36.60		-5.607		741 148	1.0	
4			N	THE		311		37.81		-4.576			1.0	
•	OTA 67 MOTA	-	CA	THE		311		38.03		-3.380		949 532	1.0	
	ATO	_	CB	THI				39.31		-2.633		303	1.0	
	OTA		OG:					39.07	-	-1.93		350	1.0	
	OTA	·			R I	311		40.46		-3.60		674	1.0	
	60 ATO	_		TH	R I	A 311		36.83	34	-2.47	J J.	5,4		. =
	UU AIU													

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5	ATOM	44	0	THR	A	311	36.021	-2.776	4.800	1.00	42.12
	ATOM	45	N	ALA	A	312	36.726	-1.372	6.409	1.00	42.16
	MOTA	46	CA	ALA	A	312	35.616	-0.444	6.228	1.00	40.10
	ATOM	47	CB	ALA	A	312	35.741	0.709	7.205	1.00	40.07
	MOTA	48	C	ALA	A	312	35.561	0.090	4.799	1.00	41.80
10	ATOM	49	Ö	ALA	A	312	34.510	0.074			
- •	ATOM	50	N	ASP	A	313			4.154	1.00	37.81
	ATOM		CA				36.698	0.564	4.304	1.00	42.35
		51		ASP	A	313	36.752	1.104	2.953	1.00	42.27
	MOTA	52	CB	ASP	A	313	38.133	1.703	2.680	1.00	43.74
1.5	ATOM	53	CG	ASP	Α	313	38.323	3.054	3.348	1.00	46.62
15	ATOM	54	OD1	ASP	A	313	39.414	3.645	3.205	1.00	51.01
	MOTA	55	OD2	ASP	A	313	37.380	3.529	4.015	1.00	48.89
	MOTA	56	С	ASP	A	313	36.422	0.027	1.926	1.00	38.68
	MOTA	57	0	ASP	A	313	35.704	0.281	0.959	1.00	38.75
	MOTA	58	N	GLN	A	314	36.931	-1.179	2.145	1.00	34.76
20	ATOM	59	CA	GLN	A	314	36.666	-2.277	1.229	1.00	33.55
	ATOM	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	36.90
	ATOM	61	CG	GLN	A	314	38.963	-3.384	1.436	1.00	40.45
	ATOM	62	CD	GLN	A	314	39.700	-4.610	1.905	1.00	43.13
	ATOM	63	OE1	GLN	A	314	39.394	-5.196	2.935	1.00	43.60
25	ATOM	64	NE2	GLN	A	314	40.701				
	ATOM	65	C	GLN	Ā	314	35.176	-5.032	1.117	1.00	44.03
	ATOM	66	0	GLN				-2.595	1.201	1.00	34.95
	ATOM	67	N	MET	A	314	34.605	-2.860	0.140	1.00	32.89
					A	315	34.542	-2.564	2.374	1.00	32.54
30	MOTA	68	CA	MET	A	315	33.115	-2.848	2.470	1.00	35.46
30	MOTA	69	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
	MOTA	70	CG	MET	A	315	31.137	-2.777	4.097	1.00	39.42
	ATOM	71	SD	MET	A	315	30.443	-4.426	4.053	1.00	46.55
	MOTA	72	CE	MET	A	315	31.351	-5.205	5.397	1.00	45.29
	ATOM	73	С	MET	A	315	32.311	-1.859	1.640	1.00	31.83
35	ATOM	74	0	MET	A	315	31.453	-2.247	0.852	1.00	32.10
	MOTA	75	N	VAL	A	316	32.587	-0.560	1.830	1.00	32.62
	MOTA	76	CA	VAL	A	316	31.882	0.470	1.079	1.00	31.09
	MOTA	77	CB	VAL	A	316	32.395	1.888	1.425	1.00	34.77
	MOTA	78	CG1	VAL	A	316	31.786	2.899	0.461	1.00	34.10
40	ATOM	79	CG2	VAL	A	316	32.021	2.246	2.862	1.00	34.40
	ATOM	80	С	VAL	A	316	32.092		-0.414	1.00	33.48
	ATOM	81	0	VAL	A	316	31.145		-1.200	1.00	32.49
	MOTA	82	N	SER	A	317	33.337	-0.027		1.00	33.49
	ATOM	83	CA	SER	A	317	33.682	-0.280			
45	ATOM	84	CB	SER	A	317	35.165			1.00	32.88
	MOTA	85	OG	SER	A	317		-0.635		1.00	35.77
	ATOM	86	C	SER			35.825		-3.154	1.00	42.70
		87			A	317	32.849	-1.396		1.00	30.71
	MOTA		0	SER	A	317	32.279	-1.238		1.00	31.14
50	MOTA	88	N	ALA	A	318	32.792	-2.529		1.00	29.51
50	MOTA	89	CA	ALA	A	318	32.035	-3.676		1.00	29.93
	MOTA	90	CB	ALA	A	318	32.156	-4.811	-1.579	1.00	28.56
	ATOM	91	С	ALA	A	318	30.565	-3.305	-2.771	1.00	31.55
	ATOM	92	0	ALA	A	318	29.961	-3.642	-3.784	1.00	30.64
	ATOM	93	N	LEU	Α	319	29.997	-2.614	-1.791	1.00	34.13
55	ATOM	94	CA	LEU	A	319	28.597	-2.212		1.00	32.93
	MOTA	95	CB	LEU	A	319	28.170	-1.576		1.00	31.15
	ATOM	96	CG	LEU	A	319	28.076	-2.555	0.632	1.00	32.27
	ATOM	97	CD1	LEU	A	319	27.523	-1.840	1.852	1.00	32.14
	ATOM	98	CD2	LEU	A	319	27.194	-3.733	0.243	1.00	31.82
60	ATOM	99	C	LEU	A	319	28.340	-1.257			
	ATOM	100	Õ	LEU	A	319				1.00	34.41
	0.1	100	9	باند	~	213	27.430	-1.475	-2.818	1.00	35.23

	WO 99/0	60014					
							29.140 -0.195 -3.120 1.00 32.53
5	ATOM	101	И	LEU		320	0 756 -4.212 1.00 35.33
ر	MOTA	102	CA	LEU		320	20.0.
	MOTA	103	CB	LEU		320	3 899 -3.054 1.00 34.60
	ATOM	104	CG	LEU		320	= === 1 00 33 69
	ATOM	105	CD1	LEU		320	31.060 3.540 3.06
10		106	CD2	LEU		320	28.611 3.302 3.5 41
10	MOTA	107	C	LEU	A	320	29.052 0.040 1.00 39 16
	MOTA	108	Ö	LEU	A	320	28.230 0.271 - 5.220 - 50 36 33
	MOTA	109	N	AASP	A	321	30.042 =0.833 = 605 0 50 35 76
	MOTA	110	N	BASP	A	321	30.041 -0.839 -3.030
. ~	MOTA	111	CA	AASP	A	321	30.214 -1.555 0.50 0.50 37.11
15	ATOM	112	CA	BASP	A	321	30.258 -1.595 -0.520
	MOTA	113	CB	AASP	A	321	31.537 -2.334 -0.575 0.50 39 41
	MOTA	114	CB	BASP		321	31.5/3 -2.3/4 0.50 0.50 41 93
	MOTA	115	CG	AASP		321	31.694 -3.230 -3.230 -3.230 -3.230 -3.230
	MOTA	115	CG	BASE		321	32.770 -1.302 7.200 0 50 42 11
20	MOTA		OD1	AASI		321	31.523 -2.733 3.355 0.50 43 43
	MOTA	117	OD1	BASI		321	33.312 -1.866 3.500 0.50 42.69
	MOTA	118		AASI		321	31.988 -4.432 3.33
	MOTA	119				321	33.170 -0.622 0.50 37 19
	MOTA	120		AAS	-	321	29.069 -2.324 -7.273
25	MOTA	121		BAS		321	29.123 -2.565 7.255
	MOTA	122		AAS		321	28.820 -2.861 0.101 0.50 36 08
	MOTA	123		BAS		321	28.934 -2.942 0.120
	ATOM	124 125	-	ALA		322	28.374 -2.968 5.225
	MOTA	123		ALA		322	27.268 -3.902 -5.125 1.00 30.73
30		12	-	ALA		322	27.124 -4.781 -3.278 -1.00 30.07
	MOTA	12		ALA	A A	322	25.946 -3.204 - 0.705 - 1.00 26 53
	MOTA	12		AL	A A	322	24.955
	MOTA MOTA	1.3		GL	J A	323	25.932 1.117 -6.827 1.00 29.88
3:		13		. GL	J A	323	24.713 -1.127 -6.855 1.00 30.98
3.	MOTA	13	-		U A		1 068 -5 509 1.00 31.62
	MOTA	13		GL.	U A		24.870
	MOTA	13) GL	A U		20 20 20 256 -4 257 1.00 33.10
	MOTA						236 -5 233 1.00 30.01
Δ	MOTA 0		36 O				04 010 -1 515 -8.123 1.00 30.86
7	ATOM		37 C	GI			705 -9 151 1.00 28.86
	ATOM		38 0				22 674 -1.659 -8.083 1.00 30.66
	ATOM		39 N				1 466 -6.935 1.00 31.01
	ATOM		40 C		RO I		21 935 -2.032 -9.290 1.00 30.29
	45 ATOM			_		A 324 A 324	20 613 -2.598 -8.760 1.00 31.42
	ATOM	1 1		_			20 626 -2.363 -7.258 1.00 33.66
	MOTA	1 1		-			21.717 -0.785-10.138 1.00 27.46
	MOTA	v 1	L44 C	-			21.893 0.332 -9.668 1.00 20.13
	OTA		L45 C			A 324 A 325	21 335 -0.959-11.403 1.00 27.00
	50 ATO			•		A 325	21.082 -2.198-12.161 1.00 27.50
	OTA					A 325	21.125 0.242-12.211 1.00 23.00
	OTA					A 325	21.258 -0.266-13.637 1.00 21.02
	OTA	• -			PRO PRO	A 325	20.773 -1.695-13.559 1.00 20.00
	OTA	•-			PRO PRO	A 32	19.749 0.830-11.954 1.00 23.73
	55 ATO			•	PRO	A 32	18 873 0.165-11.402 1.00 24.03
	ATC			_	ILE	A 32	6 19.571 2.081-12.352 1.00 22.12
	OTA				ILE	A 32	c 18 296 2.762-12.212 1.00
	ATC		154		ILE	A 32	6 18.502 4.282-12.133 1.00 20.75
)TA		155		ILE	A 32	6 17.168 4.992-12.286 1.00 29.31
	60 AT		156 157	CG2	ILE	A 32	
	ATO	ויינט	73/		•		133
							= -

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5	MOTA	158	CD1	ILE	A	326	19.301	6.120-10.525	1.00	32.91
	ATOM	159	C	ILE	A	326	17.506	2.408-13.471	1.00	25.72
	MOTA	160	0	ILE	A	326	17.906	2.758-14.581	1.00	25.55
	MOTA	161	N	LEU	A	327	16.392	1.703-13.301	1.00	25.57
	MOTA	162	CA	LEU	A	327	15.595	1.279-14.439	1.00	23.80
10	ATOM	163	CB	LEU	A	327	14.872	-0.029-14.104	1.00	23.96
	ATOM	164	CG	LEU	Α	327	15.778	-1.210-13.728	1.00	19.89
	ATOM	165	CD1	LEU	A	327	14.944	-2.462-13.583	1.00	21.19
	ATOM	166	CD2	LEU	A	327	16.850	-1.415-14.805	1.00	17.53
	ATOM	167	C	LEU	Α	327	14.598	2.317-14.935	1.00	27.16
15	ATOM	168	0	LEU	A	327	14.161	3.202-14.194	1.00	25.98
	ATOM	169	N	TYR	A	328	14.251	2.207-16.210	1.00	26.56
	ATOM	170	CA	TYR	A	328	13.303	3.123-16.814	1.00	24.45
	ATOM	171	CB	TYR	A	328	13.724	3.465-18.245	1.00	26.72
	ATOM	172	CG	TYR	A	328	14.587	4.693-18.314	1.00	27.73
20	MOTA	173	CD1	TYR .	A	328	14.021	5.949-18.518	1.00	28.56
	ATOM	174	CE1	TYR	A	328	14.798	7.092-18.509	1.00	29.10
	ATOM	175	CD2	TYR	A	328	15.962	4.612-18.110	1.00	26.01
	ATOM	176	CE2	TYR	A	328	16.750	5.753-18.098	1.00	30.63
	MOTA	177	cz	TYR	A	328	16.157	6.988-18.297	1.00	30.07
25	MOTA	178	OH	TYR	A	328	16.917	8.130-18.265	1.00	37.94
	MOTA	179	С	TYR	A	328	11.923	2.501-16.827	1.00	24.95
	ATOM	180	0	TYR	Α	328	11.774	1.274-16.846	1.00	27.02
	ATOM	181	N	SER	A	329	10.912	3.358-16.800	1.00	25.60
	MOTA	182	CA	SER	A	329	9.533	2.908-16.837	1.00	29.45
30	MOTA	183	CB	SER	A	329	8.661	3.858-16.020	1.00	30.80
	MOTA	184	OG	SER	A	329	7.297	3.721-16.364	1.00	33.74
	ATOM	185	C	SER	A	329	9.129	2.947-18.313	1.00	31.30
	MOTA	186	0	SER	A	329	9.908	3.397-19.154	1.00	27.35
0.5	ATOM	187	N	GLU	A	330	7.930	2.469-18.629	1.00	32.98
35	MOTA	188	CA	GLU	Α	330	7.459	2.482-20.007	1.00	35.10
	MOTA	189	CB	GLU	Α	330	6.031	1.968-20.074	1.00	34.67
	MOTA	190	C	GLU	A	330	7.532	3.924-20.505	1.00	40.06
	MOTA	191	0	GLU	A	330	7.068	4.841-19.826	1.00	42.65
40	MOTA	192	N	TYR	A	331	8.124	4.126-21.681	1.00	41.16
40	MOTA	193	CA	TYR	A	331	8.263	5.470-22.234	1.00	42.66
	MOTA	194	CB	TYR	A	331	9.323	5.482-23.350	1.00	42.54
	ATOM	195	CG	TYR	A	331	9.202	4.347-24.345	1.00	38.67
	MOTA	196	CD1	TYR	A	331	10.105	3.284-24.334	1.00	34.66
15	MOTA	197	CE1	TYR	Α	331	9.985	2.228-25.233	1.00	34.89
45	ATOM	198		TYR	Α	331	8.174	4.327-25.287	1.00	37.88
	MOTA	199	CE2	TYR	A	331	8.045	3.276-26.193	1.00	34.65
	MOTA	200	CZ	TYR	Α	331	8.950	2.232-26.159	1.00	30.73
	MOTA	201	OH	TYR	A	331	8.814	1.191-27.042	1.00	30.97
50	ATOM	202	С	TYR	A	331	6.943	6.043-22.754	1.00	46.24
50	MOTA	203	0	TYR	A	331	6.018	5.301-23.096	1.00	45.38
	MOTA	204	N	ASP	A	332	6.868	7.372-22.792	1.00	49.11
	ATOM	205	CA	ASP	A	332	5.684	8.092-23.262	1.00	52.40
	ATOM	206	CB	ASP	A	332	5.781	8.321-24.772	1.00	52.86
55	ATOM	207	C	ASP	A	332	4.356	7.410-22.926	1.00	52.90
55	ATOM	208	0	ASP	Α	332	3.561	7.116-23.818	1.00	53.94
	ATOM	209	N	PRO	A	333	4.103	7.144-21.632	1.00	53.63
	ATOM	210	CD	PRO	A	333	4.962	7.418-20.465	1.00	53.63
	ATOM	211	CA	PRO	A	333	2.840	6.497-21.253	1.00	53.55
60	ATOM	212	CB	PRO	A	333	3.070	6.076-19.802	1.00	53.78
60	ATOM	213	CG	PRO	A	333	4.101	7.028-19.290	1.00	53.42
	ATOM	214	С	PRO	A	333	1.673	7.478-21.398	1.00	52.17

	WO 99/0	60014					•	
							- 050	8.690-21.395 1.00 51.19
_	V	215	0	PRO	A	333	1.879	6.956-21.532 1.00 52.26
5	MOTA	216	N	THR	A	334	0.457	7.802-21.687 1.00 54.21
	MOTA	217	CA	THR	A	334	-0.724	6.949-21.813 1.00 53.90
	MOTA		CB	THR	A	334	-1.997	6.256-23.065 1.00 53.92
	MOTA	218	OG1	THR	A	334	-1.971	6.256-25.000
	MOTA	219	CG2	THR	A	334	-3.237	1.021-21
10	MOTA	220		THR	A	334	-0.864	8.762-20.525
	MOTA	221	C	THR	A	334	-1.389	0,445-45,10-
	MOTA	222	0		A	335	-0.386	10.002-20.700
	MOTA	223	N	ARG	A	335	-0.377	11.099-19.00
	ATOM	224	CA	ARG	Ā	335	-0.569	12.427-20:000
15	MOTA	225	CB	ARG		335	-1.349	10.996-10.02
	MOTA	226	С	ARG	A	335	-0.919	10.908-17.475 1.00 60.70
	MOTA	227	0	ARG	A	336	-2.667	11.015-18.889 1.00 52.43
	MOTA	228	N	PRO	A	336	-3.389	11.117-20.165 1.00 49.06
	MOTA	229	CD	PRO	A		-3.587	10.915-17.752 1.00 49.58
20	MOTA	230	CA	PRO	A	336	-4.911	11.456-18.302 1.00 48.66
_0	ATOM	231	CB	PRO	A	336	-4.645	11.809-19.760 1.00 51.33
	MOTA	232	CG	PRO	A	336	-3.698	9 468-17 279 1.00 49.25
	ATOM	233	C	PRO	Α	336	-4.340	0 644-17 929 1.00 48.06
	MOTA	234	0	PRO	A	336	-3.063	9 170-16 147 1.00 47.90
25	MOTA	235		PHE	A	337	-3.065	7 821-15.582 1.00 46.61
23	MOTA	236		PHE	A	337	-2.063	7 732-14 421 1.00 47.73
	MOTA	237		PHE	A	337	-0.649	9 011-14 805 1.00 46.27
	MOTA	238		PHE	A	337		0 168-14 368 1.00 46.55
	ATOM	239		PHE	A	337	-0.017	7 113-15 591 1.00 48.12
30		240	_	PHE	A		0.061 1.305	9 429-14 707 1.00 48.09
30	MOTA	24:			A			7 364-15.938 1.00 47.57
	MOTA	24			A		1.386	405 1 00 48 40
	ATOM	24		PHE	E A		2.009	7.238-15.071 1.00 46.15
	MOTA	24	_	PHE	3 A		-4.403	0 0 127-14 671 1.00 48.34
2		24	_	PHI	\mathbf{E} \mathbf{A}			0 8.127 15 000 1 00 45.06
3	MOTA 5	24		SE	R A			3 0.022 100 45 12
				SE	R. A			1 5.505 22 2 00 44 49
	MOTA				R I	338	-6.47	7 4.331 23 1 00 45 78
	MOTA				R I	A 338		7 3.200 201 1 00 47.04
	MOTA		50 C	SE	R A	A 338	3 -5.29	2 4.133 20 1 00 44 08
2	MOTA 04		51 0	SE		A 33	-4.09	4.186-13.507 1.00 45.63
	ATOM		52 N	GL		A 33	9 -6.20	3.910 12.000 1 00 45 40
	ATOM		53 C <i>P</i>			A 33	9 -5.80	3.012-11.000 1.00 45.66
	ATOM	-	54 CE	_		A 33	9 -7.01	15 2.521-10.621
	ATOM	-	55 CC			A 33	9 -6.63	37 1.880 3.00 47.56
	45 ATON	-	56 CI			A 33	9 -7.7	1.652 6.555
	MOTA		-	_	LՄ	A 33	9 -8.4	71 0.656 0.17
	ATO	•			ւՄ	A 33	9 -7.8	10 2.023 7.75
	ATO	-			LU	A 33	9 -5.0	40 1.621 12.270
	ATO	-	_		TΩ 	A 33	-3.8	62 1.641-11.0.2
	50 ATO				LA		₁₀ -5.7	12 1.010-12.504 1 00 40 24
	OTA	• -			LA		₁₀ -5.0	178 -0.158-15.5/1
	OTA	• •	_		LA		40 -6.0	155 -0.0/1-14.220
	ATC	• •		_	LA		40 -3.8	337 0.273-14:330
	OTA		264 C		LA		40 -2.9	909 -0.515-14.543 1.00 33.30
	55 ATC		265 C	_	ER		41 -3.8	336 1.535-14.773 1.00 33.75
	OTA		266 N	· .		_	41 -2.5	742 2.133-15.537 1.00 30.30
	OTA	MC			SER	_	41 -3.2	231 3.454 - 16.154 1.00 39.01
	TA	MC		-	SER		41 -2.2	211 4.130-16.864 1.00 36.03
	ATC				SER	_	41 -1.	480 2.376-14.691 1.00 35.63
	60 AT			_	SER			1 00 33.20
	AT		271	0	SER	A -		-
							135	

_	_									
5	ATOM	272	N	MET	A	342	-1.626	3.115-13.595	1.00	35.92
	ATOM	273	CA	MET	A	342	-0.498	3.396-12.708		
	ATOM	274	CB	\mathtt{MET}	A	342	-0.912			
	ATOM	275	CG	MET	A	342	0.241			
	MOTA	276	.SD	MET	A	342	-0.308			
10	ATOM	277	CE	MET	A	342	0.626			_
	ATOM	278	С	MET	A	342	-0.011			
	ATOM	279	0	MET	A	342	1.195			
	ATOM	280	N	MET	A	343	-0.957			_
	ATOM	281	CA	MET	A	343	-0.640			
15	MOTA	282	СВ	MET	A	343	-1.921			
	MOTA	283	CG	MET	A	343				_
	ATOM	284	SD	MET	A	343	-2.667			
	ATOM	285	CE	MET	A		-1.749	-0.507 -7.940	1.00	
	ATOM	286	C	MET		343	-1.468	-2.299 -7.886	1.00	
20	ATOM	287	0	MET	A	343	0.234	-0.875-11.979		31.72
	ATOM	288	И		A	343	1.159	-1.558-11.527		
	ATOM	289	CA	GLY	A	344	-0.069	-0.823-13.272		29.04
	ATOM	290	CA	GLY	A	344	0.688	-1.591-14.242		
	ATOM	291	0	GLY	A	344	2.104	-1.085-14.396	1.00	
25	ATOM	292	_	GLY	A	344	3.046	-1.873-14.463	1.00	
	ATOM	292	N	LEU	A	345	2.257	0.232-14.471	1.00	26.97
	ATOM	293 294	CA	LEU	A	345	3.576	0.839-14.608	1.00	31.15
	ATOM		CB	LEU	A	345	3.459	2.361-14.753	1.00	30.06
	ATOM	295	CG	LEU	A	345	2.765	2.924-15.995	1.00	33.50
30	ATOM	296	CD1	LEU	A	345	2.901	4.439-15.999	1.00	33.52
50		297	CD2	LEU	A	345	3.379	2.324-17.257	1.00	33.22
	MOTA	298	C	LEU	A	345	4.433	0.534-13.383	1.00	30.31
	MOTA	299	0	LEU	A	345	5.564	0.061-13.505	1.00	32.80
	ATOM	300	N	LEU	A	346	3.884	0.813-12.205	1.00	27.83
35	ATOM	301	CA	LEU	A	346	4.595	0.596-10.947	1.00	26.19
33	MOTA	302	CB	LEU	A	346	3.729	1.063 -9.783	1.00	24.51
	MOTA	303	CG	LEU	A	346	3.483	2.569 -9.682	1.00	26.33
	ATOM	304	CD1	LEU	Α	346	2.623	2.844 -8.463	1.00	27.33
	ATOM	305	CD2	LEU	A	346	4.809	3.317 -9.587	1.00	24.89
40	ATOM	306	С	LEU	A	346	5.032	-0.848-10.707	1.00	25.72
40	ATOM	307	0	LEU	Α	346	6.181	-1.102-10.345	1.00	29.86
	ATOM	308	N	THR	A	347	4.117	-1.793-10.891	1.00	23.80
	ATOM	309	CA	THR	A	347	4.436	-3.196-10.674	1.00	23.91
	ATOM	310	CB	THR	A	347	3.164	-4.058-10.641	1.00	26.39
15	ATOM	311	OG1	THR	A	347	2.421	-3.860-11.849	1.00	24.57
45	ATOM	312	CG2	THR	A	347	2.301	-3.682 -9.444	1.00	23.98
	ATOM	313	C	THR	A	347	5.366	-3.734-11.756	1.00	26.17
	ATOM	314	0	THR	A	347	6.176	-4.622-11.496	1.00	27.44
	MOTA	315	N	ASN	A	348	5.242	-3.197-12.970	1.00	
50	ATOM	316	CA	ASN	Α	348	6.092	-3.617-14.082	1.00	25.48
50	ATOM	317	CB	ASN	Α	348	5.657	-2.926-15.385	1.00	23.77
	ATOM	318	, CG	ASN	Α	348	6.522	-3.302-16.571	1.00	24.59
	ATOM	319	OD1	ASN	A	348	7.616	-2.799-16.771		29.93
	ATOM	320	ND2	ASN	A	348	6.010	-4.236-17.391	1.00	24.81
	ATOM	321	C	ASN	A	348	7.532	-3.229-13.741	1.00	32.61
55	ATOM	322	0	ASN	A	348	8.453	-4.027-13.870	1.00	22.82
	ATOM	323	N	LEU	A	349	7.711	-1.993-13.288	1.00	18.83
	MOTA	324	CA	LEU	A	349	9.030	-1.593-13.288	1.00	22.58
	ATOM	325	CB	LEU	A	349	8.929		1.00	21.85
	ATOM	326	CG	LEU	A	349	10.155	-0.028-12.536	1.00	22.00
60	ATOM	327	CD1	LEU	A	349	11.224	0.673-11.953	1.00	23.64
	MOTA	328	CD2	LEU	A	349	9.726	0.826-13.017	1.00	19.35
			_			- 45	3.140	2.040-11.415	1.00	21.97
						400				

	WO 33/0	00014							
					70	349		9.564	-2.335-11.734 1.00 22.94
5	ATOM	329	С	LEU	A	349	4	10.724	-2.749-11.717 1.00 23.97
_	MOTA	330	0	LEU	A	350	•	8.705	-2.591-10.756 1.00 21.67
	MOTA	331	N	ALA	A			9.113	-3.356 -9.586 1.00 21.83
	MOTA	332	CA	ALA	A	350		7.963	_3 441 -8.593 1.00 18.95
	MOTA	333	CB	ALA	A	350		9.568	-4 757 -9.985 1.00 21.90
10	MOTA	334	С	ALA	A	350			-5.221 -9.554 1.00 24.15
10		335	0	ALA	A	350		10.625	-5.423-10.810 1.00 23.24
	MOTA	336	И	ASP	Α	351		8.767	-6.772-11.259 1.00 25.87
	MOTA	337	CA	ASP	A	351		9.093	-0.//2-11.400
	MOTA	338	CB	ASP	A	351		8.028	-/.4/4-12.202
	ATOM		CG	ASP	A	351	•	8.103	-0.//2-14:10
15	MOTA	339	OD1	ASP	A	351		8.217	-9.196 13.020
	MOTA	340		ASP	A	351		8.049	-9.525-11.401
	MOTA	341	OD2	ASP	A	351		10.469	-0.023-11.510
	MOTA	342	C			35:		11.219	- / . / / 3 - 12 . / 6
	ATOM	343	0	ASP		35		10.810	-5.808-12.697 1.00 23.58
20	MOTA	344	N	ARG		35		12.115	-5.787-13.347 1.00 21.07
	MOTA	345	CA	ARG				12.120	-4.785-14.507 1.00 21.02
	MOTA	346	CB	ARC		35		11.539	-5.352-15.797 1.00 20.44
	MOTA	347	CG	ARG		35		11.554	-4.319-16.915 1.00 20.43
	ATOM	348	CD	ARC		35		10.592	2 245-16 687 1.00 19.85
25	ATOM	349	NE	ARC		35		10.910	-1 954-16.641 1.00 19.69
23	MOTA	350		AR		_		12.172	1 564-16 813 1.00 17.36
	MOTA	351		AR	G A				1 049-16 441 1.00 21.88
	ATOM	352		AR	G A			9.962	1 00 22 11
	MOTA	353		AR	G A		52	13.223	1 00 24 13
20		354		AR	G A		52	14.346	1 10 18 66
30	MOTA	35	_	GL	U A	-	53	12.909	1 00 19 08
		35	_	GI	U P	_	53	13.888	2 1 00 21.62
	MOTA	35	_	GI	υ I	4 3	53	13.317	7 = 3.102 = 3.400 = 00 20 97
	ATOM	35				3	53	13.295	2 7 7 10 10 1 20 2 3 84
	MOTA	35	-			A 3	53	12.832	2 -0.040 3.120 1 00 24 76
35		36	_			A 3	53	11.61	1 -0.531 -5.525 - 1 00 24 95
	MOTA		-			A 3	53	13.68	6 0.088 -0.557
	MOTA	36	_			A 3	53	14.24	6 -5.423 -5.512
	MOTA	36					353	15.39	8 -5.600 -5.101 200 19 54
	MOTA						354	13.24	6 -6.257 -9.255 .200 21 77
4	MOTA 0.		-		EU		354	13.43	4 - 7.452 0.110 -
	MOTA		65 CZ	-			354	12.10	07 -8.209 -8.270 1.00 23.03
	ATOM		66 CI		EU		354	11.16	50 -7.606 -7.223 1.00 23.00
	MOTA		67 C	_	EU		354	9.72	20 -8.013 -7.510 1.00 23.43
	ATOM	-			EU		354	11.58	34 -8.069 -5.839 1.00 23.31
4	45 ATOM				EU		354	14.50	00 -8.386 -8.981 1.00 23.24
	MOTA	<u>1</u> 3	70 C		EU		354	15.25	55 -9.007 -8.234 1.00 22.44
	MOTA	<u>1</u> 3	71 0		ΈU	A		14.5	60 -8.490-10.302 1.00 22.52
	IOTA	_	72 N		JAV	A	355	15.5	51 -9.343-10.935 1.00 21.66
	ATO		373 C		VAL	A	355	15.3	53 9 365-12 466 1.00 24.35
	50 ATO		374		$_{ m VAL}$	A	355	16.4	25 10 214-13 119 1.00 28.16
	ATO		375		\mathtt{VAL}	A	355		$\frac{1}{100}$ $\frac{1}{100}$ $\frac{1}{100}$ $\frac{1}{100}$
	OTA			CG2	VAL	A	355	13.9	$\frac{1}{2}$
	OTA			3	LAV	A	355	16.9	744 -0.011 -0.0 23 51
	ATO OTA				VAL	A	355	17.8	7 489-10 669 1.00 21.27
		• -		-	HIS	Α	356	17.1	105 = 7.489 = 10.000 = 100 21 31
	55 ATO			CA	HIS	A	356	18.3	392 -6.86.2-10.303 2.00 19 87
	OTA		_	CB	HIS	A	356	18.3	384 -5.390-10.011 - 1 00 21 77
	ATC			CG	HIS	A	356	18.4	494 -5.205-12.255 - 00 21 66
	ATO		•	CD2	HIS	A	356	17.5	543 -5.040 15.220 - 1 00 21 11
)TA			ND1	HIS	A	356	19.	704 -5.177-12.555 -1 00 24 96
	60 AT			CE1	HIS	A	356	19.	496 -5.011-14.249 1.00 24.96
	AT	MC	385	- L				137	
								13/	

_					_		
5	ATOM ·	386	NE2	HIS	A	356	18.192 -4.931-14.455 1.00 18.37
	MOTA	387	С	HIS	A	356	18.702 -6.947 -8.875 1.00 21.41
	MOTA	388	0	HIS	A	356	19.864 -7.111 -8.465 1.00 21.88
	MOTA	389	N	MET	A	357	17.660 -6.843 -8.058 1.00 21.84
	MOTA	390	CA	\mathtt{MET}	A	357	17.837 -6.906 -6.610 1.00 21.51
10	MOTA	391	CB	MET	A	357	16.503 -6.668 -5.898 1.00 17.60
	MOTA	392	CG	MET	A	357	16.629 -6.579 -4.369 1.00 19.36
	MOTA	393	SD	MET	A	357	15.051 -6.755 -3.531 1.00 23.64
	MOTA	394	CE	MET	Α	357	14.189 -5.332 -4.163 1.00 23.13
	MOTA	395	С	MET	A	357	18.411 -8.259 -6.192 1.00 23.69
15	ATOM	396	0	MET	Α	357	19.337 -8.328 -5.389 1.00 24.41
	MOTA	397	N	ILE	A	358	17.856 -9.331 -6.746 1.00 27.14
	MOTA	398	CA	ILE	A	358	18.314 -10.672 -6.425 1.00 28.79
	MOTA	399	CB	ILE	Α	358	17.529 -11.725 -7.232 1.00 32.42
	MOTA	400	CG2	ILE	Α	358	18.267 -13.064 -7.220 1.00 32.77
20	MOTA	401	CG1	ILE	A	358	16.125 -11.880 -6.644 1.00 31.94
	MOTA	402	CD1	ILE	A	358	15.062 -12.196 -7.680 1.00 34.85
	MOTA	403	C	ILE	Α	358	19.801 -10.802 -6.728 1.00 28.75
	MOTA	404	0	ILE	Α	358	20.569 -11.305 -5.912 1.00 31.60
	MOTA	405	N	ASN	A	359	20.207 -10.325 -7.897 1.00 27.91
25	MOTA	406	CA	ASN	Α	359	21.601 -10.401 -8.293 1.00 29.16
	ATOM	407	CB	ASN	A	359	21.721 -10.172 -9.801 1.00 31.88
	ATOM	408	CG	ASN	A	359	21.253 -11.381-10.599 1.00 39.34
	ATOM	409	OD1	ASN	A	359	21.916 -12.422-10.612 1.00 41.27
	MOTA	410	ND2	ASN	Α	359	20.102 -11.255-11.253 1.00 38.58
30	ATOM	411	С	ASN	Α	359	22.476 -9.436 -7.510 1.00 30.75
	MOTA	412	0	ASN	Α	359	23.686 -9.629 -7.412 1.00 33.35
	ATOM	413	N	TRP	A	360	21.872 -8.400 -6.940 1.00 30.07
	MOTA	414	CA	TRP	Α	360	22.634 -7.451 -6.132 1.00 27.87
	MOTA	415	CB	TRP	A	360	21.849 -6.150 -5.948 1.00 24.80
35	MOTA	416	CG	TRP	A	360	22.196 -5.392 -4.691 1.00 23.04
	MOTA	417	CD2	TRP	Α	360	21.501 -5.443 -3.438 1.00 19.83
	MOTA	418	CE2	TRP	Α	360	22.147 -4.543 -2.564 1.00 22.31
	MOTA	419	CE3	TRP	A	360	20.392 -6.165 -2.972 1.00 20.09
	MOTA	420	CD1	TRP	Α	360	23.212 -4.488 -4.529 1.00 18.99
40	MOTA	421	NE1	TRP	A	360	23.187 -3.974 -3.255 1.00 21.17
	MOTA	422	CZ2	TRP	A	360	21.721 -4.340 -1.243 1.00 20.43
	MOTA	423	CZ3	TRP	Α	360	19.968 -5.965 -1.661 1.00 20.12
	ATOM	424	CH2	TRP	Α	360	20.635 -5.057 -0.812 1.00 18.54
	MOTA	425	С	TRP	Α	360	22.892 -8.099 -4.766 1.00 24.88
45	ATOM	426	0	TRP	Α	360	23.978 -7.980 -4.198 1.00 25.00
	ATOM	427	N	ALA	A	361	21.879 -8.789 -4.252 1.00 24.08
	MOTA	428	CA	ALA	A	361	21.972 -9.462 -2.958 1.00 26.06
	MOTA	429	CB	ALA	A	361	20.676 -10.203 -2.672 1.00 20.27
	MOTA	430	С	ALA	A	361	23.161 -10.433 -2.897 1.00 28.44
50	MOTA	431	0	ALA	Α	361	23.843 -10.531 -1.876 1.00 28.95
	MOTA	432	N	LYS	A	362	23.414 -11.144 -3.992 1.00 31.41
	MOTA	433	CA	LYS	A	362	24.530 -12.097 -4.047 1.00 33.33
	MOTA	434	CB	LYS	A	362	24.564 -12.824 -5.390 1.00 34.81
- -	MOTA	435	CG	LYS	Α	362	23.319 -13.608 -5.756 1.00 36.27
55	MOTA	436	CD	LYS	A	362	23.458 -14.178 -7.167 1.00 38.30
	ATOM	437	CE	LYS	A	362	22.369 -15.193 -7.472 1.00 40.94
	MOTA	438	NZ	LYS	A	362	22.111 -15.322 -8.937 1.00 42.49
	MOTA	439	С	LYS	Α	362	25.854 -11.351 -3.893 1.00 34.17
	ATOM	440	0	LYS	A	362	26.880 -11.977 -3.595 1.00 35.40
60	ATOM	441	N	AARG		363	25.826 -10.059 -4.095 0.50 34.23
	MOTA	442	N	BARG	A	363	25.826 -10.059 -4.095 0.50 34.03

	WO 33/0	00014				
					262	27.035 -9.254 -3.987 0.50 33.25
5	ATOM	443	CA	AARG A	363	27 035 -9 254 -3.987 0.50 32.83
	ATOM	444	CA	BARG A	363	27 031 -8 153 -5.044 0.50 34.67
	ATOM	445	CB	AARG A	363	27 031 -8.153 -5.045 0.50 34.20
	ATOM	446	CB	BARG A	363	26 933 -8 654 -6.478 0.50 36.32
	MOTA	447	CG	AARG A	363	400 0 ED 35 56
10	ATOM	448	CG	BARG A	363	26.930
10	ATOM	449	CD	AARG A	363	27.745 -7.773 -7.120
		450	CD	BARG A	363	27.752 = 7.761 = 7.422 0.50 39.98
	MOTA	451	NE	AARG A	363	29.1/1 -7.73
	MOTA	452	NE	BARG A	363	27.195 = 7.725 5.752
	MOTA	452 453	CZ	AARG A	363	30.086 -7.030 7.055 0.50 40.03
15	MOTA		CZ	BARG A	363	27.905
	MOTA	454		AARG A	363	29.735
	MOTA	455	NHl	BARG A		29.205 -7.191 -9.761 0.50 40.42
	MOTA	456	NH1	AARG A		31.358 -7.123 -7.326 0.50 43.19
	MOTA	457	NH2			27.311 - 7.436 - 11.041 0.50 38.91
20	MOTA	458	NH2	BARG A		27 207 -8.630 -2.610 0.50 33.28
	MOTA	459	С	AARG A		27 207 -8.630 -2.610 0.50 32.81
	MOTA	460	C	BARG A		28 223 -7.992 -2.344 0.50 34.18
	MOTA	461	0	AARG A		28.223 -7.992 -2.345 0.50 33.43
	MOTA	462	0	BARG A		26 215 -8 798 -1.740 1.00 33.12
25	ATOM	463	N	VAL F		
23	MOTA	464	CA	VAL A		
	ATOM	465		VAL A	A 364	24.898
	MOTA	466		VAL A	A 364	25.036
	ATOM	467		VAL 3	A 364	23.946 -7.326 -7.327
30	MOTA	468		VAL	A 364	27.184
30	ATOM	469		VAL .	A 364	26.878 -10.341 0.0 36.08
	MOTA	470		PRO	A 365	28.306 -3.025 - 7.00 34.84
	MOTA	471		PRO	A 365	28.775 = 7.235 5.772 1 00 37 82
		472			A 365	29.231 -9.442 2.700
2.5	MOTA	47		PRO	A 365	30.110 -8.400 2.100
35		47	_	PRO	A 365	30.127 -7.247 1.473
	ATOM			PRO	A 365	28.538 -10.373 2.72
	MOTA	47		PRO	A 365	27.692
	MOTA	47	_	GLY	A 366	28.890 -11.654 2.651
	MOTA	47	•		A 366	28.307 -12.033 3.30
40		47	_	GLY	A 366	26.991 -13.264 3.138 1.00 39.32
	MOTA	47	-	GLY	A 366	26.638 -14.336 3.635 1.00 39.53
	MOTA	_			A 367	26.246 -12.615 2.236 1.00 38.60
	MOTA .			PHE	A 367	24.960 -13.148 1.783 1.00 36.36
	MOTA				A 367	24 291 -12 178 0.808 1.00 32.10
4	5 ATOM					22 827 -12.473 0.581 1.00 30.12
	ATOM		34 CC		·	22,401 -13.083 -0.596 1.00 28.95
	ATOM			O1 PHE		21.882 - 12.176 1.563 1.00 26.18
	MOTA	1 4		D2 PHE		21 050 -13.400 -0.792 1.00 29.42
	MOTA	1 4	-	E1 PHE	A 367	20 535 -12 491 1.373 1.00 27.60
4	OTA 05		88 C	E2 PHE	A 367	20.118 -13 103 0.196 1.00 26.81
•	OTA		89 C		A 367	1, 510 1 117 1 00 36.82
	ATO		90 C	PHE	A 367	25.0/2 14.320 1.359 1.00 36.55
	ATO		91 0	PHE	A 367	24.244 -15.390 1.303
	ATO!		92 N	VAL	A 368	3 26.088 -14.094 0.270 -1.00 42.34
	55 ATO	-		A VAL	A 368	26.289 15.903 3.11
	OTA CC			B VAL	A 368	3 27.386 -15.850 1.50 44.60
				G1 VAL	A 368	26.9/2 -14.831 2.330
	OTA	• -		G2 VAL	A 36	8 28.707 -13.437 0.010
	OTA			VAL	A 36	8 26.664 -17.100 0.533 1.00 43.65
	OTA O			VAL	A 36	8 26.469 -18.274 0.216 1.00 44.03
	60 ATC			N ASP	A 36	7 DEN 1 609 1.00 44.00
	ATC	זאַני	マンシ 1	. 1201		139

5	ATOM	500	CA	ASP	A	369	27.579 -17.755 2.688 1.00 44.96
	MOTA	501	СВ	ASP	Α	369	28.336 -17.106 3.849 1.00 43.76
	MOTA	502	CG	ASP	A	369	29.608 -16.413 3.404 1.00 43.04
	ATOM	503	OD1	ASP	A	369	30.121 -15.570 4.167 1.00 44.32
	MOTA	504	OD2	ASP	A	369	30.097 -16.709 2.293 1.00 46.76
10	ATOM	505	С	ASP	A	369	26.340 -18.465 3.228 1.00 45.89
- 0	ATOM	506	0	ASP	A	369	26.360 -19.671 3.475 1.00 48.61
	ATOM	507	N	LEU	A	370	25.261 -17.714 3.407 1.00 43.59
	MOTA	508	CA	LEU	A	370	24.020 -18.279 3.924 1.00 44.24
	ATOM	509	CB	LEU	Α	370	22.980 -17.173 4.110 1.00 41.42
15	MOTA	510	CG	LEU	A	370	23.404 -16.015 5.014 1.00 41.45
13	MOTA	511	CD1	LEU	A	370	22.219 -15.095 5.245 1.00 42.25
	ATOM	512	CD2	LEU	A	370	23.931 -16.552 6.332 1.00 38.35
	ATOM	513	C	LEU	A	370	23.449 -19.360 3.013 1.00 44.03
	ATOM	514	0	LEU	A	370	23.773 -19.423 1.829 1.00 43.63
20	ATOM	515	N	THR	A	371	22.593 -20.206 3.575 1.00 44.29
20	MOTA	516	CA	THR	A	371	21.968 -21.272 2.806 1.00 44.84
		517	CB	THR	A	371	21.29322.302 3.730 1.00 45.65
	MOTA	517	OG1	THR	A	371	20.262 -21.663 4.495 1.00 46.43
	MOTA	519	CG2	THR	A	371	22.314 -22.903 4.677 1.00 46.48
25	MOTA	520	CG2	THR	A	371	20.923 -20.684 1.864 1.00 44.93
23	MOTA	520 521	0	THR	A	371	20.418 -19.585 2.092 1.00 44.36
	ATOM	521	Ŋ	LEU	A	372	20.607 -21.418 0.804 1.00 43.83
	ATOM	522 523	CA	LEU	Ā	372	19.624 -20.971 -0.166 1.00 44.62
	MOTA	523 524	CB	LEU	Ā	372	19.407 -22.043 -1.237 1.00 47.17
20	MOTA	52 4 52 5	CG	LEU	Ā	372	18.512 -21.690 -2.429 1.00 46.91
30	MOTA			LEU	A	372	19.005 -20.417 -3.098 1.00 48.73
	MOTA	526 527	CD1 CD2	LEU	Ā	372	18.521 -22.844 -3.420 1.00 51.12
	MOTA			LEU	A	372	18.307 -20.644 0.512 1.00 44.84
	ATOM	528	С 0	LEU	A	372	17.705 -19.602 0.261 1.00 43.25
25	MOTA	529 530	N	HIS	A	372	17.849 -21.558 1.382 1.00 43.14
35	MOTA	530		HIS	Ā	373	16.599 -21.353 2.100 1.00 42.23
	MOTA	531	CA	HIS	A	373	16.318 -22.525 3.062 1.00 45.38
	MOTA	532 533	CB CG	HIS	A	373	15.114 -22.315 3.934 1.00 51.43
	MOTA	534	CD2	HIS	Ā	373	13.808 -22.621 3.743 1.00 54.99
40	MOTA	535	ND1	HIS	A	373	15.187 -21.716 5.174 1.00 54.26
40	ATOM	536	CE1	HIS	A	373	13.979 -21.663 5.709 1.00 53.77
	MOTA	537	NE2	HIS	A	373	13.124 -22.206 4.861 1.00 55.27
	MOTA		NE2	HIS	A	373	16.665 -20.047 2.885 1.00 39.78
	MOTA	538 539	0	HIS	A	373	15.677 -19.324 2.971 1.00 37.71
45	MOTA	540	N	ASP	A	374	17.839 -19.738 3.440 1.00 36.38
43	ATOM	541	CA	ASP	A	374	18.020 -18.516 4.219 1.00 37.21
	MOTA	542	CB	ASP	A	374	19.287 -18.620 5.073 1.00 38.17
	MOTA	543	CG	ASP	A	374	19.064 -19.425 6.344 1.00 41.47
	ATOM	544	OD1	ASP	A	374	17.896 -19.543 6.772 1.00 37.09
50	MOTA		OD1	ASP	A	374	20.052 -19.940 6.912 1.00 44.40
50	MOTA	545 546		ASP	A	374	18.083 -17.277 3.326 1.00 37.19
	ATOM	546	C O	ASP	A	374	17.598 -16.208 3.696 1.00 38.13
	MOTA	547		GLN			18.688 -17.431 2.152 1.00 33.13
	MOTA	548			A		18.788 -16.339 1.198 1.00 31.94
<i></i>	MOTA	549		GLN	A		19.634 -16.756 -0.001 1.00 28.81
55	MOTA	550		GLN			21.125 -16.570 0.189 1.00 31.71
	ATOM	551		GLN			21.920 -17.222 -0.922 1.00 34.49
	MOTA	552		GLN			21.478 -17.267 -2.067 1.00 36.09
	MOTA	553		GLN			23.097 -17.736 -0.588 1.00 40.32
	MOTA	554		GLN			17.379 -16.009 0.730 1.00 31.50
60		555		GLN			
	MOTA	556	0	GLN	A	375	16.990 -14.840 0.653 1.00 27.42

5	ATOM	557	N	VAL .	A	376	16.617 -17.056 0.429 1.00 30.38
5	ATOM	558	CA		A	376	15.242 -16.907 -0.027 1.00 33.50
	MOTA	559	CB		A	376	14.588 -18.286 -0.286 1.00 30.57
•	ATOM	560	CG1	•	A	376	13.093 -18.122 -0.516 1.00 33.14
	MOTA	561	CG2		Α	376	15.232 -18.952 -1.485 1.00 30.79
10	ATOM	562	C		A	376	14.393 -16.159 1.002 1.00 33.80
10	ATOM	563	0		A	376	13.653 -15.237 0.661 1.00 34.89
		564	N	HIS	A	377	14.500 -16.568 2.261 1.00 33.35
	ATOM	565	CA	HIS	A	377	13.730 -15.941 3.329 1.00 32.81
	MOTA	566	CB	HIS	A	377	13.966 -16.694 4.644 1.00 35.24
1.5	MOTA	567	CG	HIS	A	377	13.429 -15.989 5.851 1.00 40.15
15	MOTA	568	CD2	HIS	A	377	14.054 -15.495 6.946 1.00 40.86
	ATOM		ND1	HIS	A	377	12.090 -15.703 6.012 1.00 43.08
	MOTA	569	CE1	HIS	A	377	11.913 -15.062 7.154 1.00 42.44
	MOTA	570	NE2	HIS	A	377	13.089 -14.922 7.740 1.00 44.85
20	MOTA	571	NE2 C	HIS	Ā	377	14.058 -14.454 3.507 1.00 28.63
20	MOTA	572		HIS	Ā	377	13.158 -13.619 3.613 1.00 29.20
	MOTA	573	0	LEU	A	378	15.343 -14.125 3.544 1.00 24.41
	MOTA	574	N	LEU	A	378	15.759 -12.738 3.721 1.00 23.21
	MOTA	575 576	CA	LEU	A	378	17.289 -12.650 3.743 1.00 20.98
25	MOTA	576	CB	LEU	A	378	17.960 -13.190 5.016 1.00 24.22
25	MOTA	577	CG	LEU	A	378	19.471 -13.041 4.924 1.00 21.07
	MOTA	578	CD1 CD2	LEU	A	378	17.431 -12.446 6.221 1.00 20.24
	ATOM	579		LEU	A	378	15.190 -11.827 2.630 1.00 24.78
	ATOM	580	C O	LEU	A	378	14.638 -10.766 2.922 1.00 22.09
20	ATOM	581	И	LEU	A	379	15.321 -12.242 1.374 1.00 24.13
30	MOTA	582	CA	LEU	A	379	14.812 -11.447 0.262 1.00 25.02
	MOTA	583	CB	LEU	A	379	15.307 -12.025 -1.062 1.00 27.12
	MOTA	584 585	CG	LEU	Ā	379	16.724 -11.600 -1.437 1.00 24.39
	ATOM	586	CD1	LEU	A	379	17.299 -12.557 -2.470 1.00 27.58
25	MOTA	587	CD2	LEU	A	379	16.679 -10.178 -1.983 1.00 29.05
35	MOTA	588	CD2	LEU	A	379	13.287 -11.355 0.246 1.00 27.61
	MOTA	589	0	LEU	A	379	12.726 -10.301 -0.062 1.00 26.16
	MOTA	590	N	GLU	A	380	12.616 -12.454 0.576 1.00 25.65
	MOTA MOTA	591	CA	GLU	A	380	11.154 -12.471 0.592 1.00 26.85
40	MOTA	592	CB	GLU	A	380	10.640 -13.882 0.871 1.00 29.38
40	MOTA	593	CG	GLU	A	380	10.718 -14.796 -0.331 1.00 35.58
	MOTA	594		GLU	A	380	10.228 -16.194 -0.025 1.00 39.31
	ATOM	595			A	380	10.142 -17.008 -0.967 1.00 42.89
	ATOM	596			A	380	9.927 -16.478 1.153 1.00 39.45
45		597		GLU	A	380	10.604 -11.526 1.649 1.00 25.43
43	ATOM	598		GLU	A	380	9.551 -10.925 1.469 1.00 27.75
	ATOM	599		CYS	A	381	11.324 -11.400 2.753 1.00 25.57
	MOTA	600		CYS	A	381	10.907 -10.530 3.843 1.00 26.46
	ATOM	601		CYS	A		11.570 -11.000 5.149 1.00 31.46
50		602		CYS	A		11.305 -9.946 6.623 1.00 45.32
50		603		CYS	A		11.262 -9.059 3.589 1.00 24.77
	ATOM	604		CYS			10.516 -8.166 3.975 1.00 25.01
	MOTA	605		ALA			12.377 -8.815 2.903 1.00 22.23
	ATOM			ALA			12.855 -7.449 2.681 1.00 21.83
5.6	MOTA	606		ALA			14.319 -7.383 3.095 1.00 21.56
55		601		ALA			12.705 -6.778 1.311 1.00 19.78
	MOTA	608		ALA			12.996 -5.587 1.182 1.00 17.01
	MOTA	609		TRP			12.261 -7.507 0.294 1.00 17.61
	MOTA	610					12.164 -6.915 -1.036 1.00 18.06
<i>c</i>	MOTA	61					11.580 -7.928 -2.035 1.00 20.28
60		61					10.105 -8.201 -1.919 1.00 20.50
	MOTA	61	ے دن	IKE	-	. 505	

5	ATOM	614	CD2	TRP	A	383	9.049	-7.509 -2.599	3 00	22 42
J	ATOM	615	CE2	TRP	A	383	7.836	-8.138 -2.238	1.00	22.48
	ATOM	616	CE3	TRP	A	383			1.00	20.41
	ATOM	617	CD1	TRP	A	383	9.012	-6.420 -3.482	1.00	22.06
	ATOM						9.506	-9.189 -1.190	1.00	23.38
10		618	NE1	TRP	A	383	8.142	-9.159 -1.377	1.00	22.59
10	MOTA	619	CZ2	TRP	A	383	6.598	-7.713 -2.724	1.00	21.98
	ATOM	620	CZ3	TRP	A	383	7.780	-5.998 -3.968	1.00	25.50
	MOTA	621	CH2	TRP	A	383	6.589	-6.647 -3.587	1.00	23.11
	ATOM	622	C	TRP	A	383	11.448	-5.564 -1.170	1.00	19.18
1.5	MOTA	623	0	TRP	A	383	11.972	-4.663 -1.824	1.00	19.27
15	ATOM .	624	N	LEU	A	384	10.273	-5.396 -0.567	1.00	18.32
	ATOM	625	CA	LEU	A	384	9.586	-4.118 -0.719	1.00	16.38
	MOTA	626	CB	LEU	A	384	8.125	-4.218 -0.258	1.00	16.79
	ATOM	627	CG	LEU	A	384	7.211	-3.013 -0.577	1.00	18.39
20	ATOM	623	CD1	LEU	A	384	7.464	-2.485 -1.995	1.00	13.91
20	ATOM	629	CD2	LEU	A	384	5.750	-3.432 -0.410	1.00	18.38
	ATOM	630	С	LEU	A	384	10.324	-3.027 0.051	1.00	18.80
	ATOM	631	0	LEU	Α	384	10.334	-1.870 -0.357	1.00	20.90
	MOTA	632	N	${ t GLU}$	A	385	10.949	-3.404 1.163	1.00	18.61
· -	MOTA	633	CA	GLU	A	385	11.718	-2.462 1.970	1.00	19.58
25	MOTA	634	CB	GLU	A	385	12.274	-3.154 3.213	1.00	17.43
	ATOM	635	CG	GLU	A	385	11.292	-3.237 4.357	1.00	22.92
	MOTA	636	CD	GLU	A	385	11.963	-3.676 5.640	1.00	25.83
	MOTA	637	OE1	GLU	A	385	12.431	-2.799 6.391	1.00	23.69
20	MOTA	638	OE2	GLU	A	385	12.027	-4.897 5.889	1.00	27.64
30	ATOM	639	C	GLU	A	385	12.890	-1.934 1.156	1.00	19.46
	MOTA	640	0	GLU	A	385	13.206	-0.743 1.196	1.00	15.04
	MOTA	641	N	ILE	A	386	13.539	-2.842 0.431	1.00	13.32
	ATOM	642	CA.	ILE	A	386	14.685	-2.484 -0.388	1.00	15.01
25	ATOM	643	CB	ILE	A	386	15.475	-3.763 -0.807	1.00	17.43
35	ATOM	644	CG2	ILE	Α	386	16.544	-3.424 -1.849	1.00	17.99
	ATOM	645	CG1	ILE	A	386	16.185	-4.338 0.432	1.00	20.31
	ATOM	646	CD1	ILE	A	386	16.682	-5.766 0.284	1.00	23.97
	ATOM	647	C	ILE	Α	386	14.273	-1.645 -1.598	1.00	16.10
40	ATOM	648	0	ILE	A	386	14.993	-0.724 -2.004	1.00	17.42
40	MOTA	649	N	LEU	A	387	13.112	-1.944 -2.167	1.00	17.61
	ATOM	650	CA	LEU	A	387	12.620	-1.173 -3.304	1.00	18.20
	ATOM	651	CB	LEU	A	387	11.359	-1.814 -3.882	1.00	17.51
	ATOM ATOM	652	CG	LEU	A	387	11.519	-3.064 -4.747	1.00	26.37
45	ATOM	653 654	CD1	LEU	A	387	10.173	-3.406 -5.395	1.00	24.63
73		654 655	CD2	LEU	A	387	12.589	-2.824 -5.808	1.00	21.58
	ATOM ATOM	655	C	LEU	A	387	12.283	0.249 -2.838	1.00	17.60
	ATOM	656 657	O N	LEU	A	387	12.571	1.224 -3.530	1.00	17.15
	MOTA	658	N	MET	A	388	11.677	0.357 -1.660	1.00	17.65
50			CA	MET	A	388	11.286	1.656 -1.121	1.00	18.49
50	ATOM	659	CB	MET	A	388	10.302	1.460 0.034	1.00	19.65
	ATOM	660	CG	MET	A	388	8.893	1.105 -0.435	1.00	15.12
	ATOM	661	SD	MET	A	388	7.744	0.769 0.910	1.00	18.73
	MOTA	662	CE	MET	A	388	6.163	0.908 0.048	1.00	18.34
55	ATOM	663	C	MET	A	388	12.451	2.553 -0.691	1.00	22.62
"	ATOM	664	0	MET	A	388	12.417	3.767 -0.928	1.00	22.49
	ATOM	665	N	ILE	A	389	13.482	1.988 -0.064	1.00	21.45
	ATOM	666	CA	ILE	Ā	389	14.604	2.831 0.331	1.00	18.54
	ATOM	667	CB	ILE	A	389	15.590	2.108 1.299	1.00	19.35
60	ATOM	668	CG2	ILE	A	389	16.362	0.998 0.578	1.00	15.50
υU	ATOM	669	CG1		. A	389	16.556	3.142 1.889	1.00	21.95
	MOTA	670	CD1	ILE	A	389	17.373	2.658 3.080	1.00	15.86

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WO 99/060014	

	WO 99/0	60014						
					_		15.333	3.322 -0.922 1.00 18.67
5	MOTA	671	C			89	15.333	4 453 -0.970 1.00 19.75
,	ATOM	672	0	ILE		89	_	2.477 -1.943 1.00 20.58
	MOTA	673	N	GLY		90	15.410	2.895 -3.183 1.00 19.33
	MOTA	674	CA	GLY		90	16.049	4.021 -3.819 1.00 17.48
	ATOM	675	С	GLY		90	15.243	4.994 -4.318 1.00 21.87
10	ATOM	676	0	GLY		90	15.801	3.888 -3.787 1.00 19.17
10	MOTA	677	N	LEU		391	13.920	4.887 -4.343 1.00 21.50
	MOTA	678	CA	LEU		391	13.018	4.420 -4.194 1.00 18.25
	ATOM	679	CB	LEU		391	11.561	5.497 -4.342 1.00 21.98
	MOTA	680	CG	LEU		391	10.480	6.156 -5.725 1.00 21.39
15	MOTA	681	CD1	LEU		391	10.579	4.868 -4.148 1.00 17.15
13	ATOM	682	CD2	LEU		391	9.115	6.216 -3.620 1.00 23.27
	ATOM	683	C	LEU		391	13.208	7.255 -4.243 1.00 23.60
	ATOM	684	Ō	LEU	A	391	13.440	6.170 -2.295 1.00 23.04
	ATOM	685	И	VAL	A	392	13.122	7.357 -1.469 1.00 24.42
20	ATOM	686	CA	VAL	A	392	13.282	7.55, 2.00
20	MOTA	687	CB	VAL	A	392	13.186	0.555 0.000
		688	CG1	VAL	A	392	13.733 .	0.125
	MOTA	689	CG2	VAL	A	392	11.739	0.712 0.11
	MOTA	690	C	VAL	A	392	14.626	0.014 2
25	MOTA	691	0	VAL	A	392	14.728	9.242 1.002
25	MOTA	692	N	TRP	A	393	15.652	7.180 -1.521
	MOTA	693	CA	TRP	A	393	16.999	7.070 2.20
	MOTA	694		TRP	A	393	17.977	0.401 2.20
	MOTA	695		TRP	A	393	19.287	6.784 -2.857 1.00 25.90 7.605 -2.339 1.00 28.09
30	MOTA MOTA	696			A	393	20.341	7.612 -3.302 1.00 29.94
30	MOTA	697			A	393	21.375	8.335 -1.154 1.00 30.20
	ATOM	698	_		A	393	20.512	0.555 #.25
	ATOM	699			A	393	19.710	0.555 1.00 20 64
	MOTA	700			A	393	20.963	0.000 2.000 1 00 32 43
35		703		TRP	Α	393	22.566	0.525
55	ATOM	702		TRP	A	393	21.698	1 00 36 54
	ATOM	703		2 TRF	A	393	22.709	7 7.030 7 00 25 02
	MOTA	70		TRE	A	393	17.082	00 20 97
	MOTA	70	5 0	TRE		393	17.767 16.399	. = = = = = 00 23 06
40		70	6 N	ARC		394		000 1 00 25 97
• `	MOTA	70	7 CA	ARC	3 A	394	16.412 15.776	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
	MOTA	70				394	16.243	5 195 -7.024 1.00 26.05
	MOTA	70	9 CG			394	15.83	0 5 551 -8.352 1.00 22.70
	MOTA	71	.0 CD			394	14.44	5 071 -8.363 1.00 20.71
4	5 ATOM	71	1 NE			394	14.05	3 912 -7.841 1.00 21.26
•	MOTA	71				394	14.03	4 3 108 -7,267 1.00 20.09
	MOTA			II AR		394	12.78	3 544 -7.907 1.00 21.26
	MOTA	71				394	15.62	2 9 833 -5 879 1.00 23.40
	MOTA	7:	15 C	AR		394	15.88	19 10.729 -6.677 1.00 28.61
4	MOTA 05	7:	16 0	AR			14.63	18 9.924 -4.988 1.00 26.65
	MOTA	7	17 N	SE			13.77	16 11 104 -4.902 1.00 27.46
	ATOM		18 C				12.39	35 10 696 -4 382 1.00 26.70
	MOTA	7	19 C		er A		11.91	9 530 -5.029 1.00 22.95
	ATOM	1 7	20 0	-	er A		14.31	16 12.240 -4.033 1.00 31.45
	55 ATOM		21 C		ER A		13.72	26 13 324 -3.977 1.00 28.11
	ATON		22 0		ER A		15.43	27 11 986 -3.368 1.00 33.83
	ATO		23 N		ET P			61 12 954 -2.475 1.00 38.83
	ATO					396		66 12 483 -2.112 1.00 39.47
	ATO			_		396		05 11 919 -0.715 1.00 41.37
	60 ATO	M 7				A 396		
	OTA		727 5	SD M	ET 1	A 396		<u>-</u> -
							143	
						AUDETI	THITE SHEE	T (RULE 26)

5	ATOM	728	CE	MET	A	396	20 262	13 000 1 404		
	ATOM	729	C	MET	A	396	20.263	11.996 -1.404	1.00	42.84
	ATOM	730	0	MET	A	396	16.143	14.376 -3.018	1.00	40.69
	ATOM	731	И	GLU			15.637	15.316 -2.403	1.00	38.85
	ATOM	731	CA		A	397	16.794	14.526 -4.166	1.00	42.19
10	ATOM			GLU	A	397	16.971	15.831 -4.790	1.00	44.80
10	ATOM	733	CB	GLU	A	397	18.184	15.785 -5.729	1.00	46.02
		734	CG	GLU	A	397	17.883	15.189 -7.096	1.00	54.42
	MOTA	735	CD	GLU	A	397	19.117	14.665 -7.810	1.00	59.40
	ATOM	736	OE1	GLU	A	397	19.219	13.430 -7.990	1.00	60.63
15	MOTA	737	OE2	GLU	A	397	19.980	15.485 -8.19 <u>6</u>	1.00	62.71
13	ATOM	738	C	GLU	Α	397	15.735	16.322 -5.554	1.00	42.94
	ATOM	739	0	GLΰ	A	397	15.830	17.229 -6.376	1.00	44.68
	MOTA	740	N	HIS	A	398	14.579	15.728 -5.280	1.00	40.82
	ATOM	741	CA	HIS	A	398	13.342	16.118 -5.950	1.00	39.21
20	MOTA	742	CB	HIS	A	398	12.924	15.043 -6.956	1.00	39.05
20	ATOM	743	CG	HIS	A	398	13.870	14.886 -8.104	1.00	41.57
	MOTA	744	CD2	HIS	A	398	13.904	15.484 -9.318	1.00	39.28
	MOTA	745	ND1	HIS	A	398	14.940	14.017 -8.074	1.00	41.85
	MOTA	746	CE1	HIS	A	398	15.592	14.086 -9.220	1.00	40.88
25	MOTA	747	NE2	HIS	A	398	14.985	14.969 -9.993	1.00	42.30
25	ATOM	748	C	HIS	A	398	12.216	16.332 -4.944	1.00	37.04
	ATOM	749	0	HIS	A	398	11.282	15.535 -4.864	1.00	36.51
	MOTA	750	N	PRO	A	399	12.283	17.427 -4.171	1.00	39.19
	MOTA	751	CD	PRO	A	399	13.328	18.467 -4.198	1.00	35.36
20	ATOM	752	CA	PRO	A	399	11.243	17.709 -3.173	1.00	37.10
30	MOTA	753	CB	PRO	A	399	11.603	19.101 -2.654	1.00	37.86
	MOTA	754	CG	PRO	A	399	13.050	19.267 -2.963	1.00	35.83
	MOTA	755	C	PRO	A	399	9.828	17.663 -3.744	1.00	37.02
	ATOM	756	0	PRO	A	399	9.554	18.249 -4.789	1.00	38.52
25	ATOM	757	N	GLY	A	400	8.938	16.954 -3.057	1.00	33.58
35	ATOM	758	CA	GLY	A	400	7.559	16.865 -3.503	1.00	32.12
	ATOM	759	C	GLY	A	400	7.230	15.706 -4.428	1.00	32.43
	MOTA	760	0	GLY	A	400	6.063	15.344 -4.574	1.00	33.21
	ATOM	761	N	LYS	A	401	8.237	15.112 -5.055	1.00	31.35
40	ATOM	762	CA	LYS	A	401	7.972	14.007 -5.966	1.00	30.75
40	ATOM	763	CB	LYS	A	401	8.235	14.430 -7.415	1.00	35.43
	ATOM	764	CG	LYS	A	401	8.130	15.927 -7.675	1.00	35.15
	ATOM	765	CD	LYS	A	401	9.096	16.353 -8.774	1.00	36.88
	ATOM	766	CE	LYS	A	401	8.733	17.721 -9.331	1.00	36.71
45	ATOM	767	NZ	LYS	A	401	7.295	18.027 -9.116	1.00	34.22
73	MOTA	768	C	LYS	A	401	8.768	12.746 -5.677	1.00	30.97
	ATOM ATOM	769	0	LYS	A	401	9.809	12.776 -5.006	1.00	27.60
		770	N	LEU	A	402	8.256	11.635 -6.197	1.00	27.28
	MOTA	771	CA	LEU	A	402	8.889	10.334 -6.050	1.00	29.07
50	MOTA	772	CB	LEU	A	402	7.866	9.294 -5.590	1.00	22.55
30	MOTA	773	CG	LEU	A	402	7.265	9.555 -4.207	1.00	24.94
	MOTA	774	CD1	LEU	A	402	6.126	8.583 -3.937	1.00	19.32
	ATOM	775	CD2	LEU	A	402	8.355	9.416 -3.157	1.00	21.54
	ATOM	776	C	LEU	A	402	9.448	9.948 -7.414	1.00	28.78
55	MOTA	777	0	LEU	A	402	8.704	9.836 -8.389	1.00	29.98
رر	ATOM	778	N	LEU	A	403	10.761	9.770 -7.487	1.00	27.57
	MOTA	779	CA	LEU	A	403	11.393	9.400 -8.744	1.00	27.17
	MOTA	780	CB	LEU	A	403	12.825	9.937 -8.816	1.00	26.95
	MOTA	781	CG	LEU	A	403	13.401	10.027-10.238	1.00	30.42
60	MOTA	782	CD1	LEU	A	403	14.519	11.046-10.288	1.00	30.76
60	ATOM	783	CD2	LEU	A	403	13.915	8.665-10.676	1.00	33.11
	ATOM	784	C	LEU	A	403	11.419	7.891 -8.901	1.00	24.78

				- - 7	4	.03	12.428	7.257 -8.619 1.00 24.68
5	MOTA	785	_	LEU A PHE A		04	10.306	7.319 -9.344 1.00 23.11
•	MOTA	786				.04	10.239	5.881 -9.546 1.00 26.93
	MOTA	787		PHE <i>I</i> PHE <i>I</i>		104	8.826	5.470 -9.946 1.00 27.04
	MOTA	788			_	104	7.850	5.513 -8.816 1.00 27.89
	MOTA	789			-	104	7.028	6.623 -8.631 1.00 26.20
10	MOTA	790			-	404	7.750	4.444 -7.925 1.00 23.10
	MOTA	791	CE1	-		404	6.116	6.668 -7.573 1.00 25.29
	ATOM	792 793	CE2		-	404	6.845	4.481 -6.870 1.00 21.01
	MOTA	793 794	CEZ			404	6.026	5.595 -6.693 1.00 22.91
1.5	MOTA	79 4 795	C			404	11.232	5.507-10.637 1.00 26.04 4.464-10.578 1.00 27.27
15	MOTA	796	0			404	11.882	4.401 20101
	MOTA	797	И			405	11.348	6.303 ##.000
	MOTA	798	CA	ALA	A	405	12.271	0.100 100 -
	MOTA MOTA	79 <i>9</i>	CB	ALA	Α	405	11.650	5.20, 15.00
20	ATOM	800	C	ALA	A	405	12.549	7.570 =====
20	MOTA	801	0	ALA	Α	405	11.770	0.500 25.50
	MOTA	802	N	PRO	A	406	13.672	,., <u>.</u> ,
	ATOM	803	CD	PRO	A	406	14.712	0.713 21
	MOTA	804	CA	PRO	A	406	13.977	J.033 22101
25	MOTA	805	CB	PRO	A	406	15.232	0.000 201
23	MOTA	806	CG	PRO	Α	406	15.865	7.602-14.776 1.00 31.44 9.589-15.436 1.00 32.58
	MOTA	807	С	PRO	Α	406	12.820	10.796-15.507 1.00 32.58
	MOTA	808	0	PRO	A	406	12.605	8.690-16.053 1.00 32.86
	MOTA	809	N	ASN	Α	407	12.063	9.119-16.865 1.00 32.78
30	MOTA	810	CA	ASN	A	407	10.935	8.418-18.228 1.00 34.73
50	MOTA	811	CB	ASN	A	407	10.950	6.907-18.121 1.00 35.37
	MOTA	812	CG	ASN	A	407	10.884 11.189	6.317-17.077 1.00 30.24
	ATOM	813	OD1	ASN	A	407	10.486	6.268-19.215 1.00 34.08
	MOTA	814		ASN	A .	407	9.605	8.901-16.166 1.00 34.90
35	MOTA	815		ASN	A	407	8.549	8.897-16.798 1.00 36.09
	MOTA	816		ASN	A	407	9.660	8.724-14.851 1.00 33.56
	MOTA	817		LEU	A	408 408	8.452	8.544-14.061 1.00 35.59
	MOTA	818		LEU	A	408	8.141	7.062-13.851 1.00 33.81
	MOTA	819		LEU	A.	408	6.696	6.823-13.397 1.00 36.44
40		820		LEU	A A	408	5.746	7.479-14.390 1.00 34.14
	MOTA	823			A	408	6.406	5.334-13.287 1.00 32.96
	MOTA	822		LEU LEU	A	408	8.607	9.245-12.717 1.00 38.03
	MOTA	823		LEU	A	408	8.880	8.614-11.695 1.00 36.38
	MOTA	82		LEU	A	409	8.441	10.563-12.741 1.00 37.87
4:		82 82		LEU		409	8.548	3 11.395-11.553 1.00 37.95
	MOTA	82		LEU		409	9.373	3 12.636-11.877 1.00 39.52
	MOTA			LEU		409	10.023	
	MOTA MOTA					409	11.100	0 12.517 20.00
_			-			409	10.614	4 14.00% ==
50	MOTA 0			LEU		409	7.13	2 11.752 1 00 25 70
	ATOM	_		LEU		409	6.48	2 12.540 12.000 1 00 35 29
5	ATOM		_	LEU		410	6.65	4 11.201 10.000
	MOTA					410	5.29	7 11.376 3.000 1 00 29 37
	ATOM 55 ATOM		35 CB			410	4.50	3 10.277 3.223 2.00 32 75
-	MOTA CO		36 CG			410	4.64	5 9.230 10.000 - 00 16
	MOTA	-	37 CD				4.02	7.525 10.202 1 00 30 70
	MOTA		38 CD				3.95	00 3.744 11.043 1 00 35 14
	OTA		39 C	LE			5.20	7/ 12.552 5.562 5.60 36 94
	60 ATO	=	40 0	LE.	U P		6.07	0 12.211
·	ATO	-	41 N	AS	P F	411	4.14	11 13.108 38.103 1.00

_		0.4.0	~	3 CD	70	411	2	033	13.843 -6.873	1.00	35.40
5	MOTA	842	CA	ASP	A	411		733	15.341 -7.144	1.00	40.02
	MOTA	843	CB	ASP	A				15.645 -7.928	1.00	41.32
	MOTA	844	CG	ASP	A	411		471		1.00	45.03
	MOTA	845	OD1	ASP	A	411		570	14.785 -8.001	1.00	45.01
	MOTA	846	OD2	ASP	A	411		383	16.764 -8.474	1.00	36.10
10	MOTA	847	С	ASP	A	411		727	13.234 -6.179		34.08
	MOTA	848	0	ASP	A	411		033	12.395 -6.762	1.00	
	MOTA	849	И	ARG	A	412		480	13.647 -4.940	1.00	35.99
	MOTA	850	CA	ARG	A	412		375	13.099 -4.169	1.00	39.37
	MOTA	851	CB	ARG	A	412		260	13.824 -2.825	1.00	39.75
15	MOTA	852	CG	ARG	A	412		562	15.168 -2.870	1.00	40.49
	MOTA	853	CD	ARG	A	412		454	15.736 -1.465	1.00	40.65
	MOTA	854	NE	ARG	A	412		261	14.826 -0.577	1.00	37.48
	MOTA	855	CZ	ARG	A	412		574	14.855 -0.384	1.00	42.84
	MOTA	856	NH1	ARG	A	412		316	15.754 -1.024	1.00	40.82
20	MOTA	857	NH2	ARG	Α	412		150	13.986 0.438	1.00	38.32
	MOTA	858	C	ARG	A	412		034	13.108 -4.889	1.00	39.80
	MOTA	859	0	ARG	A	412		775	12.201 -4.706	1.00	39.92
	MOTA	860	N	ASN	Α	413		.198	14.119 -5.717	1.00	41.64
	MOTA	861	CA	ASN	Α	413		458	14.215 -6.440	1.00	43.19
25	MOTA	862	CB	ASN	A	413		.518	15.533 -7.210	1.00	46.44
	MOTA	863	CG	ASN	A	413		.739	16.718 -6.299	1.00	47.86
	MOTA	864	OD1	ASN	A	413		.376	16.594 -5.249	1.00	48.05
	MOTA	865	ND2	ASN	A	413		.213	17.876 -6.687	1.00	49.43
	MOTA	866	С	ASN	A	413		. 673	13.044 -7.385	1.00	41.48
30	MOTA	867	0	ASN	A	413		.792	12.567 -7.546	1.00	40.50
	MOTA	868	N	GLN	A	414		.600	12.577 -8.010	1.00	42.82
	MOTA	869	CA	GLN	A	414		.703	11.448 -8.925	1.00	44.73
	MOTA	870	CB	GLN	A	414		.585	11.307 -9.741	1.00	47.52
	MOTA	871	CG	GLN	A	414		.572	12.088-11.049		50.47
35	MOTA	872	CD	GLN	A	414		.914	12.713-11.375		53.91
	MOTA	873	OE1	GLN	A	414		.591	13.257-10.501		53.68
	MOTA	874	NE2	GLN	A	414		.309	12.637-12.641		56.91
	MOTA	875	C	GLN	A	414		.970	10.163 -8.141	1.00	43.21
	MOTA	876	0	GLN	A	414		.491	9.193 -8.682	1.00	42.33
40	MOTA	877	N	GLY	A	415		.618	10.168 -6.860		41.97
	MOTA	878	CA	GLY	A	415		.836	8.992 -6.040		40.43 40.80
	MOTA	879	С	GLY	A	415		.306	8.720 -5.804		
	MOTA	880	0	GLY	A	415		.696	7.601 -5.472		37.83 42.16
4.5	MOTA	881	N	LYS	A	416		.129	9.748 -5.978 9.613 -5.779		44.34
45	MOTA	882	CA	LYS	A	416		.566			45.65
	MOTA	883	CB	LYS	A	416		.212	10.996 -5.704		47.42
	MOTA	884	CG	LYS	A	416		.761			50.97
	ATOM	885	CD	LYS	A	416		.910			53.25
~ ^	ATOM	886	CE	LYS	A	416		.992			56.95
50	MOTA	887	NZ	LYS	A	416		.416			45.33
	MOTA	888	C	LYS	A	416		.227			46.50
	MOTA	889	0	LYS	A	416		.339			
	MOTA	890	Ŋ	CYS	A	417		.540			45.18
	ATOM	891	CA	CYS	A	417		066			46.25 49.29
55	ATOM	892	CB	CYS	A	417		.062			49.29
	ATOM	893	SG	CYS	A	417		.916			
	ATOM	894	C	CYS	A	417		3.373			47.18 46.50
	ATOM	895	0	CYS	A	417		.220			
	ATOM	896	N	VAL	A	418		1.671			
60	MOTA	897	CA	VAL	A	418		1.866			
	ATOM	898	CB	VAL	A	418	-3	3.525	3.841 -7.206	, 1.00	40.40

	WO 99/0	60014						. ,
							-3.670	2.563 -6.410 1.00 40.22
5	ATOM	899	CG1			18	-3.071	3.538 -8.634 1.00 38.03
•	MOTA	900	CG2			118	-5.441	4 714 -5.818 1.00 41.46
	MOTA	901	С	VAL		118	-4.883	5 400 -4.963 1.00 42.08
	ATOM	902	0	VAL		418	-6.559	4.036 -5.579 1.00 40.95
	MOTA	903	N	GLU		419	-7.223	4.073 -4.275 1.00 42.51
10	MOTA	904	CA	GLU		419	-8.536	3.282 -4.333 1.00 44.52
	MOTA	905	CB	GLU		419	-9.010	2 751 -2.984 1.00 50.42
	MOTA	906	CG	GLU		419	-10.413	2.168 -3.035 1.00 54.38
	MOTA	907	CD	GLU	-	419	-10.582	1 059 -3.590 1.00 54.09
	MOTA	908	OE1	GLU	A	419	-11.347	2.820 -2.516 1.00 57.90
15	MOTA	909	OE2	GLU	A	419	-6.370	3 552 -3.121 1.00 41.11
	MOTA	910	С	GLU	A	419 419	-5.955	2.393 -3.116 1.00 39.42
	MOTA	911	0	GLU	A	420	-6.129	4 419 -2.140 1.00 40.53
	MOTA	912	И	GLY	A	420	-5.346	4.049 -0.973 1.00 37.61
	MOTA	913	CA	GLY	A	420	-3.854	4.258 -1.140 1.00 37.01
20	MOTA	914	С	GLY	A	420	-3.088	4.105 -0.190 1.00 32.59
	MOTA	915	0	GLY	A.	421	-3.444	4.623 -2.350 1.00 36.21
	MOTA	916	N	MET	A	421	-2.035	4.825 -2.656 1.00 36.02
	MOTA	917	CA	MET	A A	421	-1.799	4.607 -4.160 1.00 32.84
	MOTA	918	CB	$ exttt{MET}$	A	421	-0.351	4.754 -4.617 1.00 35.82
25	MOTA	919	CG	MET	Ā	421	0.806	3.611 -3.812 1.00 35.57
	MOTA	920	SD	MET	A	421	0.881	2.294 -5.005 1.00 32.51
	MOTA	921	CE C	MET	A	421	-1.474	6.180 -2.226 1.00 34.93 6.294 -1.985 1.00 35.17
	MOTA	922		MET	A	421	-0.275	0.254 2.50-
	MOTA	923		LAV	A	422	-2.319	7.200 2.200
30		924 925		VAL	A	422	-1.823	0.520 #1.00
	MOTA	926		VAL	A	422	-2.927	9.00/ =
	MOTA	927			A	422	-3.823	9.555 -0.555
	MOTA MOTA	928				422	-2.279	10.902 1.000
35		929		IAV	A	422	-1.231	0.450 0.200 1 00 28 41
33	MOTA	930		VAL	A	422	-0.274	9.220 0.002 1 00 31 53
	ATOM	93:		GLU	J A	423	-1.803	7.670 0.572 1.00 35 99
	MOTA	93		GLU	J A	423	-1.311	7.550 1.550 1.00 40 37
	MOTA	93		GLU	J A	423	-2.190	0.354 2.72 1 00 49 41
40		93		GLU		423	-3.588	7.123
•	ATOM	93	5 CD	GL		423	-4.438	9 188 1.835 1.00 56.91
	MOTA	93					-5.349 -4.200	6 652 0.776 1.00 54.53
	MOTA	93	7 OE				0.12	7 7 043 1.886 1.00 34.83
	MOTA	93		GL.			1.00	7 7.552 2.581 1.00 31.85
4	5 ATOM	93		GL			0.36	9 6.038 1.050 1.00 30.17
	MOTA	94		IL			1.71	1 5.488 0.929 1.00 28.99
	MOTA						1.69	6 4.195 0.109 1.00 30.96
	MOTA		12 CE				3.10	8 3.588 0.068 1.00 27.20
	MOTA		43 CC				0.67	1 3.230 0.725 1.00 30.77
4	MOTA 05		44 CC				0.81	0 1.787 0.291 1.00 34.69
	MOTA					424	2.70	0 6.483 0.312 1.00 28.21
	ATOM		46 C			A 424	3.85	66 6.551 0.735 1.00 28.40
	ATOM		47 0	_		A 425	2.25	3 7.260 -0.675 1.00 27.00
	ATOM	-	48 N			A 425	3.11	19 8.253 -1.315 1.00 27.30
	55 ATOM	-	49 C			A 425	2.38	8.958 -2.458 1.00 26.30
	MOTA	-	_	_		A 425	2.53	38 8.289 -3.798 1.00 27.22
	MOTA	_	_			A 425	2.63	19 9.030 1.00 1 27 89
	IOTA					A 425	2.5	0.500 5.55
	ATOI					A 425	2.7	21 0.445 0.501 - 00 27 28
	60 ATO					A 425		68 6.282 -5.149 1.00 27.28
	OTA	147	,,,,				1 17	

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5	MOTA	956	CZ		A	425		ਦੇ 3 ਓਹੀ। - 9.306	0.303		27.63 25.66
	MOTA	957	C	PHE	A	425	3.591	9.306 -			26.33
	MOTA	958	0	PHE	A	425	4.757				20.33 27.92
	MOTA	959	N	ASP	A	426	2.680				
	MOTA	960	CA	ASP	Α	426	2.984		1.570	1.00	28.88
10	MOTA	961	CB	ASP	A	426	1.721		2.369	1.00	32.58
	MOTA	962	CG	ASP	A	426	0.781	12.034	1.613	1.00	37.47
	ATOM	963	OD1	ASP	A	426	-0.432	12.039	1.925	1.00	37.72
	ATOM	964	OD2	ASP	A	426	1.253	12.758	0.710	1.00	36.35
	ATOM	965	С	ASP	A	426	4.071	10.278	2.532	1.00	26.96
15	ATOM	966	0	ASP	Α	426	4.974	11.030	2.900	1.00	27.20
	MOTA	967	N	MET	Α	427	3.978	9.022	2.947	1.00	25.76
	MOTA	968	CA	MET	A	427	4.981	8.468	3.856	1.00	25.89
	MOTA	969	CB	MET	Α	427	4.567	7.070	4.309	1.00	21.17
	MOTA	970	CG	MET	A	427	3.385	7.072	5.257	1.00	24.38
20	MOTA	971	SD	MET	A	427	3.153	5.489	6.080	1.00	34.32
20	ATOM	972	CE	MET	A	427	2.173	4.637	4.910	1.00	21.03
	MOTA	973	C	MET	Α	427	6.321	8.410	3.128	1.00	22.29
	ATOM	974	Ō	MET	Α	427	7.363	8.760	3.689	1.00	22.19
	ATOM	975	N	LEU	Α	428	6.285	7.985	1.868	1.00	21.75
25	MOTA	976	CA	LEU	A	428	7.506	7.892	1.075	1.00	22.91
25	MOTA	977	CB	LEU	A	428	7.202	7.252	-0.287	1.00	18.47
	MOTA	978	CG	LEU	A	428	6.910	5.747	-0.176	1.00	19.24
	MOTA	979	CD1	LEU	A	428	6.278	5.222	-1.468	1.00	16.82
	ATOM	980	CD2	LEU	A	428	8.204	5.010	0.131	1.00	16.23
30	ATOM	981	C	LEU	A	428	8.148	9.269	0.902	1.00	23.98
30	ATOM	982	0	LEU	A	428	9.366	9.416	1.034	1.00	23.06
	ATOM	983	N	LEU	A	429	7.328	10.281	0.628	1.00	23.91
	ATOM	984	CA	LEU	A	429	7.837	11.642	0.462	1.00	26.29
	MOTA	985	CB	LEU	A	429	6.714	12.571	-0.003	1.00	27.47
35	ATOM	986	CG	LEU	A	429	6.331	12.411		1.00	30.78
33	MOTA	987	CD1	LEU	A	429	5.022	13.139		1.00	34.75
	MOTA	988	CD2	LEU	A	429	7.449	12.952	-2.350	1.00	31.96
	ATOM	989	C	LEU	A	429	8.425	12.166	1.776	1.00	25.83
	ATOM	990	0	LEU	A	429	9.482	12.808	1.793	1.00	26.42
40	MOTA	991	N	ALA	A	430	7.734	11.890	2.877	1.00	26.45
40	MOTA	992	CA	ALA	A	430	8.201	12.333	4.185	1.00	26.11
	ATOM	993	CB	ALA	A	430	7.214	11.909	5.265	1.00	23.13
	MOTA	994	C	ALA	A	430	9.577	11.742	4.462	1.00	25.01
	MOTA	995	Ö	ALA	A	430	10.455	12.409	5.005	1.00	24.31
45	ATOM	996	N	THR	A	431	9.767	10.486	4.074	1.00	25.25
15	ATOM	997	CA	THR	Α	431	11.046	9.825	4.294	1.00	22.78
	ATOM	998	CB	THR	Α	431	10.973	8.323	3.962	1.00	21.36
	ATOM	999	OG1	THR	Α	431	9.924	7.727	4.727	1.00	20.27
	ATOM	100		THR	A	431	12.291		4.299	1.00	
50	MOTA	100		• THR	A	431	12.103		3.429	1.00	23.73
50	MOTA	100		THR	A		13.234		3.868	1.00	19.60
	MOTA	100		SER	A		11.736			1.00	24.32
	MOTA	100		SER	A		12.676			1.00	26.96
	ATOM	100		SER			12.067		-0.093	1.00	28.70
55		100		SER			13.084		-1.039		33.42
23		100		SER			13.033				27.92
	MOTA	100		SER			14.176				
	ATOM			SER			12.045				
	MOTA	100		SER			12.269				
۲۸	MOTA	101		SER			10.957				
60		101		SER			10.175				
	MOTA	101	.2 00	JEK	A	. =33					

5	ATOM	1013	С	SER	A	433	13.263				33.43
3	ATOM	1014	0		A	433	14.152				31.94
		1015	N		A	434	13.105	13.545	4.959		31.32
	MOTA MOTA	1015	CA	ARG	A	434	13.980	13.236	6.086		29.78
		1017	CB	ARG	A	434	13.468	11.994	6.819		29.84
10	MOTA	1017	CG	ARG	A	434	14.331	11.541	7.983		32.17
10	MOTA	1018	CD	ARG	A	434	14.626	12.672	8.958	1.00	37.00
	ATOM	1019	NE	ARG	A	434	15.321	12.169 1	0.140	1.00	39.44
	MOTA	1020	CZ	ARG	A	434	15.935	12.935	1.034	1.00	44.06
	MOTA	1021	NH1	ARG	A	434	15.949	14.255	LO.885	1.00	45.52
1.5	MOTA	1023	NH2	ARG	A	434	16.528	12.381	L2.084	1.00	45.01
15	MOTA	1023	C	ARG	A	434	15.413	13.014	5.605	1.00	29.24
	MOTA	1024	0	ARG	A	434	16.352	13.563	6.173	1.00	29.72
	ATOM	1025	N	PHE	A	435	15.577	12.206	4.561	1.00	28.95
	MOTA	1026	CA	PHE	A	435	16.901	11.935	4.000	1.00	30.59
20	MOTA	1027	CB	PHE	A	435	16.777	11.045	2.758	1.00	32.03
20	MOTA	1028	CG	PHE	A	435	16.795	9.563	3.051	1.00	31.88
	MOTA		CD1	PHE	A	435	16.758	9.084	4.359	1.00	35.60
	ATOM	1030	CD1	PHE	A	435	16.847	8.643	2.009	1.00	35.89
	MOTA	1031	CE1	PHE	A	435	16.771	7.709	4.622	1.00	35.36
26	MOTA	1032 1033		PHE	A	435	16.860	7.271	2.262	1.00	32.71
25	MOTA	1033		PHE	A	435	16.821	6.807	3.570	1.00	33.24
	MOTA	1034		PHE	A	435	17.576	13.253	3.607	1.00	32.73
	MOTA	1035		PHE	A	435	18.763	13.464	3.871	1.00	31.16
	MOTA	1036		ARG	A	436	16.812	14.137	2.975	1.00	33.37
20	MOTA	1037		ARG	A	436	17.341	15.429	2.549	1.00	39.13
30	MOTA	1036		ARG	A	436	16.282	16.206	1.756	1.00	40.42
	MOTA MOTA	1040		ARG	A	436	16.846	17.317	0.877	1.00	43.09
		1040		ARG	A	436	15.750	17.960	0.040	1.00	44.53
	MOTA MOTA	1042		ARG	A	436	14.826		-0.472	1.00	48.34
35	MOTA	1043		ARG	A	436	13.530	16.913	-0.184	1.00	48.81
33	MOTA	1044			Α	436	12.997	17.823	0.619	1.00	47.80
	MOTA	104			A	436	12.769	15.950	-0.687		49.53
	MOTA	104		ARG	A	436	17.792	16.250	3.753		38.10
	MOTA	104		ARG	A	436	18.896				41.00
40	ATOM	104		MET	A	437	16.936				39.47
40	MOTA	104		MET	A	437	17.257	17.087			38.20
	ATOM	105		MET	A	437	16.102	16.998			39.79
	MOTA	105		MET	A	437	18.550	16.594			
	MOTA	105		MET	A	437	19.303				
45		105		MET	A	438	18.804				
	ATOM	105		MET	A	438	20.01				
	ATOM	105		MET	A	438	19.787				
	MOTA	105		MET	A	438	18.694				_
	MOTA	105		MET	Α	438	18.747				
50		105		MET	Α	438	20.374				
50	ATOM	105		MET	A	438	21.17				
	MOTA	106		MET	A	438	22.32				
	MOTA	106		ASN	A	439	20.88				
	ATOM	106				439	21.92				
55		106				439	23.01				
	MOTA	106					23.93				
	MOTA	106					23.52				
	MOTA	100					25.19				
	MOTA	100		ASN			22.55				
60		10		ASI			23.76				
50	MOTA		69 N	LEU		440	21.69	2 12.69	8 3.70	4 1.0	31.47

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5	ATOM ·	1070	CA	LEU	A	440	22.161	11.326	3.579	1.00	31.63
	ATOM	1071	CB	LEU	A	440	20.991	10.344	3.380	1.00	33.05
	MOTA	1072	CG	LEU	A	440	21.451	8.886	3.209	1.00	37.07
	ATOM	1073	CD1	LEU	A	440	21.957	8.353	4.546	1.00	36.18
	ATOM	1074	CD2	LEU	A	440	20.318	8.032	2.682	1.00	32.33
10	ATOM	1075	С	LEU	A	440	23.146	11.161	2.435	1.00	32.10
	MOTA	1076	0	LEU	A	440	22.925	11.671	1.333	1.00	32.76
	MOTA	1077	N	GLN	A	441	24.225	10.450	2.702	1.00	32.54
	MOTA	1078	CA	GLN	A	441	25.255	10.220	1.699	1.00	31.97
	MOTA	1079	CB	GLN	A	441	26.632	10.320	2.345	1.00	31.75
15	MOTA	1080	CG	${ t GLN}$	A	441	26.896	11.669	2.979	1.00	35.56
	ATOM	1081	CD	${ t GLN}$	Α	441	27.040	12.748	1.939	1.00	34.97
	MOTA	1082	OE1	GLN	A	441	27.985	12.782	1.167	1.00	35.51
	MOTA	1083	NE2	GLN	A	441	26.053	13.659	1.899	1.00	35.41
	MOTA	1084	С	GLN	A	441	25.100	8.860	1.038	1.00	34.08
20	ATOM	1085	0	${\tt GLN}$	A	441	24.540	7.931	1.625	1.00	30.73
	ATOM	1086	N	GLY	A	442	25.608		-0.187	1.00	32.78
	ATOM	1087	CA	\mathtt{GLY}	A	442	25.528		-0.921	1.00	32.91
	ATOM	1088	C	GLY	A	442	26.181		-0.184	1.00	31.87
	ATOM	1089	0	GLY	Α	442	25.642		-0.154	1.00	33.18
25	MOTA	1090	N	GLU	A	443	27.340	6.603	0.416	1.00	30.60
	MOTA	1091	CA	GLU	A	443	28.057	5.567	1.150	1.00	30.85
	ATOM	1092	CB	GLU	A	443	29.376	6.111	1.704	1.00	32.74
	ATOM	1093	CG	GLU	A	443	30.425	6.378	0.646	1.00	36.30
	ATOM	1094	CD	GLU	A	443	30.310	7.770	0.066	1.00	40.92
30	ATOM	1095	OE1	GLU	A	443	29.677	8.630	0.716	1.00	42.27
	ATOM	1096	OE2	GLU	A	443	30.853		-1.038	1.00	46.82
	MOTA	1097	C	GLU	A	443	27.206	5.048	2.299	1.00	30.43
	ATOM	1098	Ö	GLU	A	443	27.211	3.854	2.595	1.00	28.11
	MOTA	1099	N	GLU	A	444	26.482	5.955	2.948	1.00	30.26
35	MOTA	1100	CA	GLU	A	444	25.619	5.589	4.067	1.00	28.18
	MOTA	1101	CB	GLU	A	444	25.147	6.843	4.797	1.00	26.32
	ATOM	1102	CG	GLU	A	444	26.250	7.633	5.463	1.00	29.27
	ATOM	1103	CD	GLU	A	444	25.748	8.944	6.023	1.00	29.62
	ATOM	1104	OE1	GLU	A	444	25.006	9.652	5.304	1.00	32.00
40	MOTA	1105	OE2	GLU	A	444	26.088	9.268	7.182	1.00	29.02
	MOTA	1106	C	GLU	A	444	24.403	4.813	3.572	1.00	26.93
	ATOM	1107	0	GLU	A	444	23.970	3.841	4.191	1.00	24.78
-	MOTA	1108	N	PHE	A	445	23.861	5.256	2.443		27.79
	ATOM	1109	CA	PHE	A	445	22.688	4.633	1.853	1.00	24.50
45	ATOM	1110	CB	PHE	A	445	22.254	5.416	0.610	1.00	25.40
	ATOM	1111	CG	PHE	A	445	21.372		-0.316	1.00	23.74
	MOTA	1112	CD1	PHE	A	445	20.034		-0.004	1.00	23.00
	MOTA	1113	CD2	PHE	A	445	21.885		-1.489	1.00	22.37
	MOTA	1114	CE1	PHE	A	445	19.215		-0.855	1.00	22.57
50	ATOM	1115	CE2	PHE	Ā	445	21.079		-2.342		
50	MOTA	1116	CZ	PHE	A	445	19.741		-2.342	1.00	21.69 22.25
	ATOM	1117	C	PHE	A	445		3.169		1.00	
	MOTA		-				22.913		1.489	1.00	22.81
	ATOM	1118 1119	N O	PHE VAL	A N	445	22.083	2.316	1.796	1.00	22.92
55	ATOM				A	446	24.019	2.868	0.822	1.00	22.46
,,		1120		VAL	A	446	24.278	1.481	0.447	1.00	22.26
	ATOM	1121		VAL	A	446	25.522		-0.465	1.00	22.87
	ATOM	1122		VAL	A	446	25.251		-1.799	1.00	22.57
	ATOM	1123		VAL	A	446	26.735	1.968	0.217	1.00	22.38
60	MOTA	1124		VAL	A	446	24.467	0.614	1.694	1.00	23.68
υυ	MOTA	1125		VAL	A	446	24.177	-0.586	1.680	1.00	22.91
	MOTA	1126	IA	CYS	A	447	24.962	1.223	2.770	1.00	22.02

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	WO 99/0	60014											. ٠
								4	0.503	4.025	1.00	24.	17
£	MOTA	1127	CA	CYS	A	447		155	1.359	5.011	1.00	23.	
5	ATOM		CB	CYS	A	447		953	1.324	4.731	1.00	28.	
	MOTA		SG	CYS	A	447		. 738	0.178	4.618	1.00	21.	
		1130	C	CYS	A	447		.781	-0.960	5.002	1.00	19.	37
	MOTA	1131	0	CYS	A	447		.512		4.680	1.00		
	MOTA	1132	И	LEU	A	448		.915	1.186	5.219	1.00		31
10	MOTA	1133	CA	LEU	A	448		.568	1.002	5.207	1.00		
	ATOM	1134	CB	LEU	A	448		.803	2.324	6.303	1.00		
	MOTA	1134	CG	LEU	Α	448		.142	3.337	6.072	1.00		
	MOTA	1135	CD1	LEU	A	448		.328	4.594	7.672	1.00		.03
	ATOM		CD2	LEU	A	448		.827	2.760				.72
15	MOTA	1137	CDZ	LEU	A	448		766	-0.038	4.442			.87
	MOTA	1138	0	LEU	A	448	20	0.006	-0.803	5.030			.42
	MOTA	1139	И	LYS	A	449	2	0.929	-0.055				.98
	MOTA	1140		LYS	A	449	2	0.205	-0.997				.55
	MOTA	1141	CA	LYS	A	449		0.440	-0.659	0.788			.82
20	MOTA	1142		LYS	A	449	1	9.438	-1.297	-0.173	1.0 2 1.0		3.33
	MOTA	1143		LYS	A	449		9.456	-0.613	-1.542	_		3.58
	MOTA	1144		LYS	A	449	2	0.816	-0.754	-2.22	9 1.0		3.77
	MOTA	1145		LYS		449	_	0.741		2 -3.69	8 1.0		0.33
	MOTA	1146		LYS		449		0.629	-2.43			-	0.57
25	MOTA	1147		LYS		449		9.800	-3.34			-	9.25
	MOTA	1148		SER		450		21.924	-2.63				1.84
	ATOM	1149		SEF	-			22.451	-3.96				0.59
	MOTA	115		SEF				23.982	-3.95				9.78
	MOTA	115		SEI	_			24.460	-3.97				1.58
30		115		SEI				21.975	-4.40			_	0.06
	MOTA	115		SE			0	21.728		0 4.68	-		2.20
	MOTA	115		IL	-			21.853	3 -3.44				2.82
	MOTA	115		IL		_		21.385	5 -3.74				L9.62
	MOTA	115		IL				21.452					21.11
3.		115			-	45		20.593					22.20
	MOTA	115		_		A 45		22.90					24.48
	MOTA	115				A 45		23.11					21.82
	MOTA	116	_	II		A 45		19.95	2 -4.2				21.72
	MOTA			II		A 45		19.57					20.18
4	MOTA 0.	11					52	19.15					18.13
	ATOM	_	63 N				52	17.76	3 -4.0				19.72
	ATOM		64 CA 65 CE	-	LE	-	52	17.02	4 -3.1			.00	18.99
	. ATOM	_			LE	_	52	15.72	20 -3.7			.00	18.33
	MOTA	•			LE		52	16.72	25 -1.7	-		.00	23.25
4	45 ATOM	-		_	LE	-	52	16.28			_	00	19.50
	MOTA				LE		52	17.72		-		00	17.60
	MOTA				LE		52	16.9		-		1.00	19.23
	IOTA	-			EU		153	18.5	55 -5.			1.00	21.60
	ATO	-		_	EU		153	18.5	89 -7.	_	-	1.00	21.50
	50 ATO				LEU		153	19.6	24 -7.		_	1.00	25.06
	ATO			_	LEU		453	19.8				1.00	25.27
	OTA		_	-	LEU		453	18.5			-		24.73
	ATO				LEU		453	20.9	48 -8.			1.00	19.41
	ATC	-	_		LEU		453	18.9	906 -8.			1.00	20.75
	55 ATC		177	-	LEU		453	18.1	L98 -9.	_		1.00	21.35
	OTA		.178		LEU		454	19.9	966 -7.	-	.499	1.00	23.67
	ATO		.179 N		LEU		454	20.4	410 -8		.530	1.00	20.69
	OTA				LEU	A	454	21.	870 -8		.878	1.00	24.92
	ATO	-			LEU	A	454	22.	816 -8		.673	1.00	24.32
	60 AT				LEU	A	454	24.		.268 6	.132	1.00	44.41
	TA	OM :	1183	CD1	200	••		1					
							15	ı					

5	B COM	1304	CD2	LEU	7\	454	22 705	-9.913	4.952	1.00	22.84
3	MOTA	1184 1185	CD2	LEU	A A	454	22.785 19.572	-8.945	7.807	1.00	26.06
	MOTA MOTA	1186	0	LEU	A	454	19.572	-9.997	8.438	1.00	27.44
			N	ASN	A	455	19.413	-7.795	8.167	1.00	25.01
	ATOM	1187								1.00	26.10
10	ATOM	1188	CA	ASN	A	455	18.240	-7.681	9.400		20.10
10	ATOM	1189	CB	ASN	A	455	18.439	-6.295		1.00	
	ATOM	1190	CG	ASN	A	455	17.627	-6.109		1.00	26.67
	MOTA	1191	OD1	ASN	A	455	17.899		12.270	1.00	25.16 20.73
	ATOM	1192	ND2	ASN	A	455	16.615		11.212	1.00	
1.5	ATOM	1193	C	ASN	A	455	16.739	-7.957	9.418	1.00	25.78
15	ATOM	1194	0	ASN	A	455	16.230		10.380	1.00	29.22
	ATOM	1195	N	SER	A	456	16.027	-7.549	8.381	1.00	28.51
	ATOM	1196	CA	SER	A	456	14.578	-7.704	8.371	1.00	32.52
	MOTA	1197	CB	SER	A	456	14.019	-7.213	7.033	1.00	35.98
20	MOTA	1198	OG ~	SER	A	456	14.266	-5.818	6.897	1.00	30.88
20	MOTA	1199	C	SER	A	456	14.033	-9.086	8.711	1.00	33.00
	MOTA	1200	0	SER	A	456	13.112	-9.202	9.523	1.00	33.07
	ATOM	1201	N	GLY	A	457		10.130	8.117	1.00	28.40
	MOTA	1202	CA	GLY	A	457	14.115	-11.464	8.413	1.00	36.28
25	ATOM	1203	C	GLY	A	457	15.055	-12.289	9.277	1.00	40.41
25	MOTA	1204	0	GLY	A	457	14.831	-13.486	9.456	1.00	38.20
	MOTA	1205	И	VAL	A	458	16.095	-11.657	9.820	1.00	44.13
	MOTA	1206	CA	VAL	A	458	17.079	-12.356		1.00	51.09
	MOTA	1207	CB	VAL	A	458	18.214	-11.399		1.00	51.06
20	ATOM	1208	CG1	VAL	A	458	17.688	-10.390		1.00	51.75
30	MOTA	1209	CG2	VAL	A	458	19.365	-12.199		1.00	50.65
	ATOM	1210	С	VAL	A	458	16.513	-13.060		1.00	57.26
	MOTA	1211	0	VAL	A	458	17.085	-14.045		1.00	58.77
	ATOM	1212	N	TYR	A	459	15.401	-12.560		1.00	62.31
25	ATOM	1213	CA	TYR	A	459	14.793	-13.177		1.00	68.49
35	MOTA	1214	CB	TYR	A	459	14.293	-12.100		1.00	70.46
	ATOM	1215	CG	TYR	A	459	15.396	-11.196		1.00	71.73
	MOTA	1216	CD1	TYR	A A	459	15.127		15.462 15.898	1.00	71.93
	MOTA	1217	CE1	TYR		459 450	16.147			1.00	72.60
40	MOTA	1218	CD2 CE2	TYR TYR	A A	459	16.716 17.741	-11.644		1.00	72.77 73.55
40	MOTA MOTA	1219	CEZ		A	459		-10.812	15.941	1.00	72.93
	ATOM	1220 1221	OH	TYR TYR	A	459 459	17.450			1.00	74.56
	ATOM	1221					18.467	-8.687	16.351	1.00	74.36
	ATOM	1223	С 0	TYR TYR	A	459 459	13.849			1.00	73.11
45	ATOM	1223		THR	A A	460		-13.756		1.00	74.84
43	ATOM	1225		THR	A	460	11.881			1.00	77.66
	ATOM	1225		THR	A	460	11.246			1.00	76.69
	MOTA	1227		THR	A	460		-15.938		1.00	80.26
	ATOM	1228		THR	A	460		-16.866		1.00	80.82
50	ATOM	1229		PHE	A	461	13.762			1.00	82.69
50	ATOM	1230		PHE	A	461		-17.299		1.00	85.63
	ATOM	1230		PHE	A	461		-17.034		1.00	85.47
	ATOM	1231		PHE	A	461		-18.288		1.00	87.52
	ATOM	1232		PHE	A	461		-18.286		1.00	86.53
55	ATOM	1233		LEU	A	461		-17.940		1.00	89.49
55	ATOM									1.00	
		1235		LEU	A 7	462 463	13.711				91.34 91.23
	MOTA	1236		LEU LEU	A n	462 463	12.961			1.00	91.23
	MOTA MOTA	1237 1238		LEU	A.	462 462		-21.060		1.00	91.91
60	ATOM	1238		SER	A A	462		-21.165			91.91
00	ATOM	1239		SER	A A	463		-21.357		1.00 1.00	92.53
	PT OM	1240	CA	SER	A	703	10.131	-21.855	10.000	1.00	24.30

	WO 99/00	00014			
		- 0.42 CD	SER A	463	16.033 -21.483 16.833 1.00 91.67
5	ATOM .	1241 CB	SER A	463	16.189 -23.371 15.200 1.00 93.39
	MOTA	1242 C		463	15.156 -24.034 15.102 1.00 93.44
	MOTA	1243 0	-	464	17.399 -23.917 15.167 1.00 93.82
	MOTA	1244 N		464	17 577 -25 355 15.015 1.00 93.85
	MOTA	1245 CA	SER A	464	17 284 -25 769 13.577 1.00 93.74
10	MOTA	1246 CB	SER A	464	10 997 -25 743 15.396 1.00 93.96
	MOTA	1247 C	SER A	464	19 815 -26 074 14.535 1.00 93.65
	MOTA	1248 O	SER A	465	10 279 -25 699 16.694 1.00 93.91
	ATOM	1249 N	THR A		20 600 -26.036 17.212 1.00 93.79
	MOTA	1250 CA	THR A	465	20 952 -27.483 16.863 1.00 93.38
15	MOTA	1251 CB	THR A	465	21.640 -25.085 16.634 1.00 93.27
	MOTA	1252 C	THR A	465	21.302 -24.017 16.121 1.00 93.03
	MOTA	1253 0	THR A	465	22.907 -25.479 16.723 1.00 93.26
	MOTA	1254 N	LEU A	466	23.999 -24.665 16.207 1.00 92.34
	MOTA	1255 CA	LEU A	466	25.335 -25.338 16.498 1.00 91.59
20	ATOM	1256 CB	LEU A	466	23.829 -24.461 14.706 1.00 92.18
	ATOM	1257 C	LEU A	466	23.829 -24.401 11.7-1
	MOTA	1258 0	LEU A	466	24.411 -23.313 -1.00 91 28
	MOTA	1259 N	LYS A	467	23.028 -23.323 21.00
	MOTA	1260 CA	LYS A	467	22.772 23.200 200 20 03
25	MOTA	1261 CB	LYS A	467	21.740 -20.207 22.00 00 35
	ATOM	1262 C	LYS A	467	22.209 23.012 1100 00 00 00
	MOTA	1263 0	LYS A		23.032 -22.330 22.03
	MOTA	1264 N	SER A		20.981 -23.010 12.00
	ATOM	1265 CA	SER A		20.384 -22.313 22.113
30	MOTA	1266 CB	SER A		18.901 -22.555 12.025 1 00 83 03
50	MOTA	1267 OG	SER A		18.229 -23.376 22.00
	ATOM	1268 C	SER A		21.109 -21.250 15.00
	ATOM	1269 0	SER P		21.264 -20.103 11.00 92 04
	MOTA	1270 N	LEU A		21.550 -21.575
35	MOTA	1271 CA	LEU <i>I</i>		22.276 -20.020 20.00 70 81
55	ATOM	1272 CB	LEU A	469	22.595 -21.254 10.100 100 70 10
	MOTA	1273 C	LEU Z	469	23.564 -20.174 11. 756 7 00 79 61
	MOTA	1274 0	LEU	A 469	24.111 -13.122 -1.11
	MOTA	1275 N	GLU 2	A 470	24.044 -20.000 20 1 00 74 84
40		1276 CA	GLU :	A 470	25.256 -20.050 -2.1 00 74 12
-10	MOTA	1277 CE	GLU .	A 470	75.003 -41.000 10.00
	ATOM	1278 C	GLU	A 470	24.920 -19.363 11.63.
	MOTA	1279 0	GLU	A 470	25.617 -10.000 11.00
	MOTA	1280 N	${ t GLU}$	A 471	23.642 -15.752 20.55
4:		1281 C	A GLU	A 471	23.396 -10.042 3.316 77 53
٦.	ATOM	1282 CI	3 GLU	A 471	22.461 -13.320 0.51
	ATOM	1283 C	GLU	A 471	23.150 -13.37 - 020 1 00 74 01
	MOTA	1284 C	D GLU	A 471	24.512 -20.500 , 15.5
	MOTA	-	E1 GLU	A 471	25.469 -20.230 7.130 - 00 75 19
5	MOTA 0		E2 GLU	A 471	24.020 -21.333 3.00 (7.33
,	MOTA	1287 C		A 471	22.667 -17.652 2600
	ATOM			A 471	21.005 -17.105 100-
	ATOM			A 472	23,154 -17,519 12,000
	MOTA		A LYS	A 472	22.564 -10.225 -2.0
_			B LYS	A 472	21.697 -10.777 13.71
3	55 ATOM		G LYS	A 472	20.683 -13.776 14.225 - 1 00 60 73
	MOTA		D LYS	A 472	19.2/1 -18.542 14.223
	ATOM		E LYS	A 472	18.485 -15.909 15.449 1.00 61.78
	ATOM		IZ LYS	A 472	19.352 -15.788 16.658 1.00 60.09
	MOTA			A 472	23.662 -15.339 13.150 1.00 53.42
,	60 ATOM	•		A 472	
	MOTA	1 1297 (D LYS		

ATOM 1299 CA ASP A 473 25.732 -1 ATOM 1300 CB ASP A 473 26.613 -1 ATOM 1301 CG ASP A 473 26.380 -1 ATOM 1302 OD1 ASP A 473 25.272 -1 10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	5.949 13.830 1.00 47.52 5.194 14.405 1.00 45.55 6.094 15.269 1.00 50.48 5.885 16.749 1.00 55.50 5.436 17.118 1.00 58.06 6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 37.25 4.904 11.026 1.00 35.07 5.523 8.653 1.00 37.36
ATOM 1300 CB ASP A 473 26.613 -1 ATOM 1301 CG ASP A 473 26.380 -1 ATOM 1302 OD1 ASP A 473 25.272 -1 10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	6.094 15.269 1.00 50.48 5.885 16.749 1.00 55.50 5.436 17.118 1.00 58.06 6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
ATOM 1300 CB ASP A 473 26.613 -1 ATOM 1301 CG ASP A 473 26.380 -1 ATOM 1302 OD1 ASP A 473 25.272 -1 10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	5.885 16.749 1.00 55.50 5.436 17.118 1.00 58.06 6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 37.36 5.523 8.653 1.00 37.36
ATOM 1301 CG ASP A 473 26.380 -1 ATOM 1302 OD1 ASP A 473 25.272 -1 10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	5.885 16.749 1.00 55.50 5.436 17.118 1.00 58.06 6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 37.36 5.523 8.653 1.00 37.36
ATOM 1302 OD1 ASP A 473 25.272 -1 10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	5.436 17.118 1.00 58.06 6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
10 ATOM 1303 OD2 ASP A 473 27.304 -1 ATOM 1304 C ASP A 473 26.557 -1	6.170 17.541 1.00 59.81 4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
ATOM 1304 C ASP A 473 26.557 -1	4.611 13.269 1.00 42.62 3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
	3.506 13.373 1.00 42.10 5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
	5.364 12.180 1.00 38.05 4.904 11.026 1.00 37.25 5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
	4.90411.0261.0037.255.9789.9411.0035.075.5238.6531.0037.36
	5.978 9.941 1.00 35.07 5.523 8.653 1.00 37.36
	5.523 8.653 1.00 37.36
	5.113 8.355 1.00 38.86
ATOM 1311 ND1 HIS A 474 27.322 -1	5.452 7.476 1.00 41.31
ATOM 1312 CE1 HIS A 474 28.110 -1	5.020 6.509 1.00 40.86
20 ATOM 1313 NE2 HIS A 474 29.311 -3	4.807 7.016 1.00 44.49
	.3.640 10.493 1.00 36.68
	2.676 10.132 1.00 36.48
	.3.652 10.447 1.00 35.93
	2.499 9.963 1.00 36.21
	2.797 9.868 1.00 36.31
	11.527 9.513 1.00 38.19
	13.874 8.813 1.00 36.97
	14.454 8.869 1.00 35.59
	11.322 10.907 1.00 35.34
	10.189 10.471 1.00 33.20
	11.596 12.206 1.00 35.95
	10.540 13.193 1.00 35.06
	11.062 14.585 1.00 37.30
	11.068 14.860 1.00 43.06
	10.051 15.017 1.00 43.93
	12.230 14.968 1.00 45.60
	11.928 15.177 1.00 47.56
	10.613 15.211 1.00 46.21
	-9.966 13.170 1.00 35.40
40 ATOM 1333 O HIS A 476 26.634	-8.774 13.415 1.00 35.45
ATOM 1334 N ARG A 477 27.420 -	10.805 12.862 1.00 34.07
	10.331 12.795 1.00 34.18
ATOM 1336 CB ARG A 477 29.757 -	11.506 12.605 1.00 41.04
ATOM 1337 CG ARG A 477 29.800 -	12.459 13.788 1.00 47.61
	13.599 13.557 1.00 55.67
	13.675 14.622 1.00 60.17
	12.811 14.770 1.00 61.98
	11.803 13.918 1.00 64.29
	12.955 15.766 1.00 62.79
	-9.361 11.621 1.00 30.77
* - *	-8.268 11.753 1.00 33.59
	-9.766 10.475 1.00 27.65
ATOM 1346 CA VAL A 478 28.389	
ATOM 1347 CB VAL A 478 27.658	
55 ATOM 1348 CG1 VAL A 478 27.672	-8.678 6.890 1.00 25.83
	10.933 7.761 1.00 31.66
ATOM 1350 C VAL A 478 27.689	-7.610 9.584 1.00 26.92
ATOM 1351 O VAL A 478 28.216	-6.536 9.294 1.00 26.9
ATOM 1352 N LEU A 479 26.499	-7.702 10.171 1.00 25.74
60 ATOM 1353 CA LEU A 479 25.727	-6.516 10.530 1.00 27.9°
ATOM 1354 CB LEU A 479 24.474	-6.912 11.324 1.00 25.55

5	MOTA	1355	CG	LEU	A	479	23.211					29.01
,	MOTA			LEU	A	479	22.056					27.05
	ATOM				A	479	22.864			_		24.92
	ATOM				A	479	26.592					25.39
	MOTA			LEU	A	479	26.595					27.39
10	MOTA		N	ASP	A	480	27.324			2.320		26.04
10	ATOM	_	CA	ASP	A	480	28.206	-5.3	88 1	3.193	1.00	27.32
	MOTA		CB	ASP	A	480	28.878	-6.3	05 1	4.222	1.00	26.67
	MOTA	1363	CG	ASP	A	480	27.990	-6.6	02 1	5.417	1.00	31.02
	ATOM	1364	OD1	ASP	A	480	28.35	-7.5	05 1	6.198	1.00	31.50
1.5	ATOM	1365	OD2	ASP	A	480	26.93	5 -5.9	44 1	5.580	1.00	32.21
15	MOTA	1366	C	ASP	A	480	29.28		99 1	2.361	1.00	25.59
		1367	0	ASP	A	480	29.67	2 -3.5	62 1	2.636	1.00	27.15
	MOTA	1368	И	LYS	A	481	29.76		94 1	1.340	1.00	25.17
	MOTA	1369	CA	LYS	A	481	30.79		30 1	0.477	1.00	24.93
20	MOTA	1370	CB	LYS	A	481	31.30		90	9.512	1.00	28.42
20	MOTA		CG	LYS	A	481	32.15		53 1	0.188	1.00	35.59
	ATOM	1371	CD	LYS	A	481	32.89			9.157	1.00	41.21
	ATOM	1372	CE	LYS	A	481	33.88		963	8.350	1.00	41.48
	MOTA	1373	NZ	LYS	A	481	34.95			9.215	1.00	43.22
25	MOTA	1374	C	LYS	A	481	30.26			9.696	1.00	26.12
25	MOTA	1375	0	LYS	A	481	30.97			9.463	1.00	23.73
	ATOM	1376	И	ILE	A	482	28.99			9.291	1.00	25.44
	MOTA	1377 1378		ILE	A	482	28.42			8.545	1.00	27.69
	MOTA		CA CB	ILE	Ā	482	27.06			7.915	1.00	27.59
20	MOTA	1379	CG2	ILE	A	482	26.47			7.183	1.00	25.97
30	MOTA	1380	CG2	ILE	A	482	27.27			6.922	1.00	23.80
	MOTA	1381	CD1	ILE	A	482	26.00			6.533	1.00	21.30
	ATOM	1382	CDI	ILE	A	482	28.25			9.481	1.00	27.33
	MOTA	1383 1384		ILE	A	482	28.3			9.045	1.00	28.55
2.5	MOTA			THR	A	483	28.04			10.768	1.00	25.03
35	ATOM	1385		THR	A	483	27.9			11.760	1.00	23.62
	MOTA	1386 1387		THR	A	483	27.5			13.154	1.00	22.18
	MOTA	1388		THR	A	483	26.1			13.133	1.00	25.39
	MOTA	1389		THR	A	483	27.6			14.226	1.00	25.84
40	MOTA	1390		THR	A	483	29.2		074	11.858	1.00	23.04
40	MOTA	1391		THR	A	483	29.3			11.846	1.00	23.55
	ATOM	1392		ASP	A	484	30.3	24 -0.	714	11.960	1.00	22.24
	MOTA	1393		ASP	A	484	31.6			12.039	1.00	
	MOTA	1394		ASP	A	484	32.7			12.107		26.88
15	MOTA	1395		ASP	A	484	32.6			13.394		32.52
45		1396		ASP	A	484	32.0			14.366		33.68
	MOTA	139		ASP	A	484	33.1			13.434		34.63
	MOTA	1398		ASP	A	484	31.9		.715	10.807	1.00	25.16
	MOTA	139		ASP		484	32.4			10.905		26.05
50	MOTA	140		THR			31.5		.226			28.96
50				THR			31.6		.960			26.63
	MOTA	140: 140:		THR			31.1		.166		1.00	26.12
	MOTA						31.7		.123		1.00	24.30
	MOTA	140					31.3		.907			23.31
	ATOM	140		THR			30.9		.318			28.90
55		140					31.5		.354			
	MOTA	140		THR LEU			29.		.310			
	MOTA	140					28.9		.537			
	ATOM	140		LEU			27.		.233			
	MOTA	140		LEU			26.		.921			
60		141							.550			
	MOTA	141	.1 CD1	L LEU	J A	. 400	، و د من					

5	MOTA	1412	CD2	LEU	A	486	26.309	4.128	7.577	1.00	21.35
	MOTA	1413	С	LEU	A	486	29.662	4.519	9.960	1.00	27.36
	MOTA	1414	0	LEU	A	486	29.745	5.710	9.669	1.00	25.87
	MOTA	1415	N	ILE	Α	487	30.151	4.015 1		1.00	27.88
	ATOM	1416	CA	ILE	A	487	30.843	4.857 1	.2.055	1.00	28.40
10	MOTA	1417	CB	ILE	A	487	31.203	4.054 1	.3.332	1.00	26.74
	MOTA	1418	CG2	ILE	A	487	32.255	4.803 1	4.154	1.00	27.54
	MOTA	1419	CG1	ILE	Α	487	29.937	3.813 1	.4.163	1.00	25.93
	MOTA	1420	CD1	ILE	A	487	29.237	5.088 1	4.624	1.00	23.42
	MOTA	1421	С	ILE	A	487	32.125	5.393 1	.1.412	1.00	28.89
15	MOTA	1422	0	ILE	A	487	32.497	6.554 1	1.602	1.00	29.85
	MOTA	1423	N	HIS	A	488	32.791	4.533 1	.0.649	1.00	29.71
	MOTA	1424	CA	HIS	A	488	34.031	4.898	9.967	1.00	34.12
	MOTA	1425	CB	HIS	A	488	34.585	3.691	9.207	1.00	36.61
	MOTA	1426	CG	HIS	A	488	35.799	3.997	8.385	1.00	42.74
20	MOTA	1427	CD2	HIS	A	488	35.970	4.089	7.045	1.00	43.12
	MOTA	1428	ND1	HIS	A	488	37.034	4.239	8.946	1.00	43.13
	ATOM	1429	CE1	HIS	A	488	37.913	4.466	7.987	1.00	43.40
	ATOM	1430	NE2	HIS	A	488	37.293	4.381	6.825	1.00	45.63
	MOTA	1431	С	HIS	A	488	33.799	6.051	8.998	1.00	32.74
25	MOTA	1432	0	HIS	A	488	34.577	7.004	8.955	1.00	31.06
	MOTA	1433	N	LEU	A	489	32.721	5.958	8.223	1.00	33.56
	MOTA	1434	CA	LEU	A	489	32.384	6.992	7.258	1.00	30.78
	MOTA	1435	CB	LEU	A	489	31.145	6.587	6.464	1.00	34.67
	MOTA	1436	CG	LEU	A	489	31.310	5.353	5.574	1.00	34.73
30	MOTA	1437	CD1	LEU	Α	489	29.945	4.856	5.125	1.00	33.21
	MOTA	1438	CD2	LEU	A	489	32.183	5.701	4.378	1.00	35.92
	MOTA	1439	С	LEU	A	489	32.124	8.320	7.954	1.00	33.97
	MOTA	1440	0	LEU	Α	489	32.587	9.365	7.507	1.00	33.22
	MOTA	1441	N	MET	A	490	31.387	8.274	9.058	1.00	31.33
35	MOTA	1442	CA	MET	Α	490	31.056	9.482	9.801	1.00	30.61
	MOTA	1443	CB	MET	A	490	30.000	9.161	10.862	1.00	32.34
	MOTA	1444	CG	MET	A	490	28.607	8.940	10.289	1.00	30.71
	MOTA	1445	SD	MET	Α	490	27.457	8.247	11.496	1.00	31.14
	MOTA	1446	CE	MET	A	490	26.321	7.408	10.418	1.00	30.36
40	MOTA	1447	С	MET	A	490	32.287	10.108	10.455	1.00	32.22
	MOTA	1448	0	MET	A	490	32.412	11.330	10.517	1.00	28.25
	ATOM	1449	И	ALA	A	491	33.184	9.262	10.949	1.00	33.81
	MOTA	1450	CA	ALA	A	491	34.407	9.730	11.585	1.00	39.92
	MOTA	1451	CB	ALA	A	491	35.168	8.554	12.185	1.00	37.22
45	MOTA	1452	С	ALA	A	491	35.275	10.445	10.550	1.00	42.68
	MOTA	1453	0	ALA	Α	491	35.865	11.487	10.838	1.00	45.32
	MOTA	1454	N	LYS	A	492	35.339	9.876	9.347	1.00	44.39
	MOTA	1455	CA	LYS	A	492	36.122	10.440	8.248	1.00	44.80
	MOTA	1456	CB	LYS	Α	492	36.136	9.477	7.052	1.00	46.96
50	MOTA	1457	CG	LYS	A	492	37.490	8.840	6.744	1.00	47.20
	MOTA	1458	CD	LYS	A	492	37.390	7.830	5.595	1.00	45.71
	MOTA	1459	CE	LYS	A	492	38.631	6.937	5.518	1.00	45.55
	ATOM	1460	NZ	LYS	Α	492	38.357	5.577	4.948	1.00	36.28
	ATOM	1461	С	LYS	Α	492	35.534	11.780	7.809	1.00	45.61
55	ATOM	1462	0	LYS	A	492	36.227	12.604	7.215	1.00	46.18
	MOTA	1463	N	ALA	Α	493	34.254	11.992	8.100	1.00	43.75
	MOTA	1464	CA	ALA	Α	493	33.590	13.238	7.728	1.00	42.42
	ATOM	1465	CB	ALA	Α	493	32.097	13.001	7.528	1.00	40.92
	ATOM	1466	С	ALA	A	493	33.816	14.305	8.796	1.00	41.78
60	MOTA	1467	0	ALA	Α	493	33.277	15.410	8.707	1.00	40.76
	MOTA	1468	N	GLY	A	494	34.604	13.960	9.811	1.00	41.01

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_		1460	C) N	GLY	A	494	34.903	14.904 10.873 1.00 41.63	
5	ATOM	1469	CA	GLY	A	494	33.857	15.060 11.965 1.00 41.18	
	MOTA	1470	C 0	GLY	A	494	33.916	16.011 12.747 1.00 38.22	
	MOTA	1471		LEU	A	495	32.905	14.138 12.043 1.00 39.53	
	MOTA	1472	N	LEU	A	495	31.876	14.248 13.068 1.00 38.91	
	MOTA	1473	CA	LEU	A	495	30.713	13.304 12.769 1.00 39.20	
10	MOTA	1474	CB		A	495	29.540	13.901 11.988 1.00 40.73	
	MOTA	1475	CG	LEU	A	495	29.976	14.170 10.553 1.00 37.80	
	MOTA	1476	CD1	LEU	A	495	28.349	12.943 12.026 1.00 40.94	
	MOTA	1477	CD2		A	495	32.461	13.923 14.431 1.00 36.01	
	MOTA	1478	C	LEU	A	495	33.347	13.074 14.544 1.00 34.85	
15	MOTA	1479	0	LEU	A	496	31.979	14.604 15.459 1.00 37.52	
	MOTA	1480	N	THR THR	A	496	32.462	14.350 16.812 1.00 35.45	
	MOTA	1481	CA	THR	A	496	31.925	15.375 17.829 1.00 37.55	
	MOTA	1482	CB	THR	Ā	496	30.498	15.263 17.908 1.00 32.93	
	MOTA	1483		THR	A	496	32.315	16.797 17.434 1.00 36.16	
20	MOTA	1484		THR	Ā	496	31.933	12.987 17.210 1.00 35.67	
	MOTA	1485		THR	Ā	496	31.081	12.427 16.521 1.00 34.34	
	MOTA	1486		LEU	Ā	497	32.429	12.452 18.319 1.00 34.88	
	MOTA	1487		LEU	A	497	31.965	11.151 18.786 1.00 35.67	
~-	ATOM	1488		LEU	A	497	32.689	10.760 20.074 1.00 41.10	
25	ATOM	1489		LEU	A	497	33.714	9.640 19.896 1.00 45.27	
	MOTA	1490			A	497	34.755	9.692 21.008 1.00 45.09	
	MOTA	1491			A	497	32.988	8.305 19.884 1.00 47.77	
	ATOM	1492		LEU	A	497	30.455	11.198 19.026 1.00 33.72	
20	MOTA	149: 149:		LEU	A	497	29.712	10.350 18.534 1.00 33.20	
30	MOTA	149		GLN	A	498	30.006	12.202 19.773 1.00 30.82	
	MOTA	149	_	GLN	A	498	28.586	12.348 20.062 1.00 31.47	
	MOTA	149		GLN	A	498	28.344	13.566 20.951 1.00 30.51	
	MOTA	149		GLN		498	26.894	13.796 21.341 1.00 34.38	
25	MOTA MOTA	149		GLN		498	26.712	15.130 22.015 1.00 38.60	
35		150				498	27.363	16.112 21.686 1.00 42.92	
	MOTA MOTA	150				498	25.809	15.176 23.008 1.00 40.02	
	MOTA	150		GLN		498	27.776	12.476 18.773 1.00 30.47	
	MOTA	150		GLN		498	26.682	11.927 18.665 1.00 30.85	
40		150		GLN		499	28.311	13.196 17.793 1.00 29.52	
70	ATOM	150		GLN	I A	499	27.603		
	ATOM	150			J A	499	28.292		
	ATOM	150				499	28.13		
	MOTA	150				499	28.93		
45		150		:1 GLM	A 7	499	29.95	0 10.515 11.11	
	ATOM	153		2 GL	A I	499	28.45	, 10.005 15.00	
	ATOM	153		GLI	A D	499	27.52	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	
	ATOM	15		GLI	7 A		26.56	7 11.755 15 15 15 15 15 15	
	MOTA	15		GL	N A		28.55		
50		15		A GL	N A		28.57	, 5,55, E5,55, 5,00, 31 E'	
•	ATOM	15		3 GL	n P		29.93		
	MOTA	15	16 C	GL:	n P		31.01	2 3.003 40.00 24 9/	
	ATOM	15	17 C	D GL	n A		32.37	= = = = = 00 26 45	
	MOTA			E1 GL	N Z	A 500	32.61	.2 0.131 10.000 - 00 20 21	
5:				E2 GL		4 500	33.30	1 10.000 00 27 9	
	MOTA	15	20 C	GL	N A	A 500	27.45	,,,	
	MOTA		21 0	GL	N I	A 500	26.70	0.405 11.500 1.00 00 0	
	MOTA	15	22 N			A 501	27.35	0.001 17.011	
	ATOM			A HI		A 501	26.32	., 0.022 2.00	
6	MOTA 0			B HI		A 501	26.53	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	
-	ATOM	15	525 C	G HI	S	A 501	27.89	92 7.420 19.535 1.00 34.2	-

5	ATOM	1526	CD2	HIS	A	501	:	28.726	6.540			36.10
-	ATOM	1527	ND1	HIS	Α	501		28.541	7.844 2		1.00	31.81
	MOTA	1528	CE1	HIS	A	501	:	29.716	7.244 2		1.00	34.89
	ATOM	1529	NE2	HIS	A	501		29.854	6.448		1.00	37.46
	ATOM	1530	C	HIS	A	501		24.935	8.572		1.00	24.93
10	ATOM	1531	0	HIS	Α	501		23.998	7.815		1.00	26.73
	MOTA	1532	N	GLN	Α	502		24.796	9.892		1.00	22.79
	MOTA	1533	CA	GLN	A	502		23.504	10.498		1.00	26.14
	MOTA	1534	CB	GLN	Α	502		23.554	12.006		1.00	22.36
	MOTA	1535	CG	GLN	A	502		23.460	12.378		1.00	26.19
15	MOTA	1536	CD	${ t GLN}$	A	502		23.589	13.875		1.00	28.67
	MOTA	1537	OE1	${ t GLN}$	Α	502		23.632	14.663		1.00	28.40
	MOTA	1538	NE2	GLN	A	502		23.651	14.268		1.00	24.72
	ATOM	1539	C	GLN	A	502		23.056	10.221		1.00	26.19
	MOTA	1540	0	GLN	A	502		21.913		15.453	1.00	24.09
20	MOTA	1541	N	ARG	A	503		23.955	10.429		1.00	24.88
	MOTA	1542		ARG	A	503		23.630	10.196		1.00	25.25 27.63
	MOTA	1543	CB	ARG	A	503		24.772	10.668		1.00 1.00	
	MOTA	1544	CG	ARG	A	503		24.432	10.563		1.00	28.75 27.72
	MOTA	1545	CD	ARG	A	503		25.479	11.222		1.00	29.35
25	MOTA	1546	NE	ARG	A	503		25.072	11.214 12.126	8.654 8.105	1.00	25.84
	MOTA	1547	CZ	ARG	A	503		24.279	13.120	8.840	1.00	27.35
	ATOM	1548	NH1	ARG	A	503		23.804	12.044	6.820	1.00	30.63
	MOTA	1549	NH2	ARG	A	503		23.347		13.065	1.00	24.53
20	MOTA	1550	C	ARG	A	503 503		22.425		12.321	1.00	25.90
30	ATOM	1551	0	ARG LEU	A A	504		24.143		13.672	1.00	23.00
	MOTA	1552	N CA	LEU	A	504		23.953		13.496	1.00	22.60
	MOTA	1553 1554		LEU	A	504		24.971		14.323	1.00	25.43
	MOTA MOTA	1555		LEU	A	504		24.781		14.344	1.00	25.23
35	MOTA	1556		LEU	A	504		25.166	3.505	12.991	.1.00	28.52
55	ATOM	1557		LEU	A	504		25.627	3.495	15.444	1.00	22.14
	ATOM	1558		LEU	A	504		22.541	6.030	13.934	1.00	22.84
	ATOM	1559		LEU	Α	504		21.846		13.245	1.00	21.51
	MOTA	1560	N	ALA	A	505		22,120		15.083	1.00	20.16
40	MOTA	1561	. CA	ALA	. A	505		20.784		15.585	1.00	21.08
	MOTA	1562	CB	ALA	Α	505		20.605		16.980	1.00	23.57
	MOTA	1563	C	ALA	Α	505		19.738		14.628	1.00	20.20
	MOTA	1564	1 0	ALA	Α	505		18.754		14.293	1.00	
	ATOM	1565	5 N	${\tt GLN}$	A	506		19.954		14.184		
45	MOTA	1566		${ t GLN}$	A	506		19.013		. 13.277		
	MOTA	1567		GLN	A	506		19.502		12.903	1.00	
	MOTA	1568		GLN	A	506		19.240		13.975		
	ATOM	1569		GLN				20.187		3 13.857 1 12.777		
	MOTA	1570		GLN				20.704		14.968		
50		157		GLN				20.423		12.016		
	ATOM	157		GLN				18.813		12.010		
	MOTA	157		GLN				17.684		11.474		
	ATOM	157		LEU				19.905 19.827		7 10.263		
~ ~	ATOM	157		LEU				21.231				
55		157		LEU				22.026				
	ATOM	157		LEU				23.371				
	ATOM	157						23.371				
	ATOM	157		LEU LEU				19.090		9 10.496		
۷۸	MOTA	158 158		LEU				18.242				
60	ATOM ATOM	158		LEU				19.402		9 11.592		
	AIOM	100	4V			. 500						

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5	MOTA	1583	CA	LEU	A	508	18.755	3.260 11.881	1.00	20.72
	ATOM		CB	LEU	A	508	19.501	2.535 13.001	1.00	22.29
	ATOM	1585	CG	LEU	A	508	20.977	2.311 12.678	1.00	24.70
	MOTA	1586	CD1	LEU	A	508	21.642	1.551 13.814	1.00	21.37
	ATOM	1587	CD2	LEU	A	508	21.095	1.542 11.367	1.00	27.88
10	ATOM	1588	С	LEU	Α	508	17.279	3.396 12.239	1.00	19.14
	ATOM	1589	0	LEU	A	508	16.498	2.478 12.003	1.00	17.80
	MOTA	1590	N	LEU	A	509	16.895	4.530 12.815	1.00	19.23
	MOTA	1591	CA	LEU	A	509	15.495	4.747 13.173	1.00	20.14
	ATOM	1592	CB	LEU	Α	509	15.347	6.030 13.999	1.00	20.28
15	ATOM	1593	CG	LEU	A	509	15.710	5.858 15.479	1.00	21.35
10	MOTA	1594	CD1	LEU	A	509	15.354	7.106 16.263	1.00	19.29
	ATOM	1595	CD2	LEU	A	509	14.989	4.656 16.038	1.00	20.84
	MOTA	1596	C	LEU	Α	509	14.681	4.841 11.885	1.00	21.69
	MOTA	1597	0	LEU	A	509	13.493	4.514 11.854	1.00	22.40
20	MOTA	1598	N	ILE	Α	510	15.343	5.270 10.815	1.00	20.22
20	ATOM	1599	CA	ILE	A	510	14.710	5.397 9.508	1.00	20.40
	ATOM	1600	CB	ILE	A	510	15.720	5.946 8.464	1.00	28.34
	ATOM	1601	CG2	ILE	A	510	15.208	5.710 7.056	1.00	32.54
	MOTA	1602	CG1	ILE	A	510	15.965	7.438 8.696	1.00	28.23
25	MOTA	1603	CD1	ILE	A	510	14.789	8.189 9.288	1.00	33.16
23	ATOM	1604	C	ILE	A	510	14.210	4.025 9.049	1.00	23.21
	ATOM	1605	Ö	ILE	A	510	13.120	3.906 8.474	1.00	21.16
	MOTA	1606	N	LEU	A	511	14.998	2.989 9.323	1.00	18.38
	ATOM	1607	CA	LEU	A	511	14.633	1.634 8.917	1.00	20.10
30	ATOM	1608	CB	LEU	A	511	15.754	0.656 9.267	1.00	21.69
50	ATOM	1609	CG	LEU	A	511	17.128	1.022 8.692	1.00	26.03
	ATOM	1610	CD1	LEU	A	511	18.024	-0.206 8.724	1.00	22.68
	ATOM	1611	CD2	LEU	A	511	16.996	1.544 7.267	1.00	26.00
	MOTA	1612	С	LEU	A	511	13.326	1.181 9.543	1.00	18.51
35	ATOM	1613	0	LEU	A	511	12.663	0.283 9.025		17.40
	MOTA	1614	N	SER	A	512	12.963	1.799 10.664		18.68
	MOTA	1615	CA	SER	A	512	11.718	1.471 11.331		18.67
	MOTA	1616	CB	SER	A	512	11.661	2.117 12.720		18.58
	MOTA	1617	OG	SER	A	512	10.315	2.229 13.165		27.92
40	ATOM	1618	C	SER	A	512	10.572	1.994 10.464		18.43
	MOTA	1619	0	SER	A	512	9.584	1.296 10.236		13.91
	MOTA	1620	N	HIS	A	513	10.713	3.228 9.982		18.95
	MOTA	1621	CA	HIS	A	513	9.698	3.831 9.124		20.82
	MOTA	1622		HIS	A	513	10.013	5.315 8.894		24.36
45	MOTA	1623		HIS	A	513	9.923	6.146 10.136		32.13
	MOTA	1624		HIS	A	513	8.863	6.744 10.734		35.29
	MOTA	1625		HIS	A	513	11.010	6.391 10.949		35.00
	MOTA	1626		HIS	A	513	10.624	7.101 11.995		34.67
	MOTA	1627		HIS	A	513	9.326	7.328 11.889		35.82
50	ATOM	1628		HIS	A	513	9.650	3.079 7.790		19.08
	MOTA	1629		HIS	A		8.575	2.863 7.220		_
	MOTA	1630	N	ILE	Α		10.809	2.662 7.29		
	ATOM	1633	L CA	ILE	A		10.849	1.921 6.038		
	MOTA	1632		ILE			12.312	1.678 5.576		
55	MOTA	1633	3 CG2				12.349	0.602 4.49		
	MOTA	1634	4 CG1				12.891	2.986 5.019		
	MOTA	1635	5 CD1				14.393	2.992 4.87		
	MOTA	163	6 C	ILE			10.112	0.590 6.21		
	ATOM	163		ILE			9.364	0.164 5.32		
60	MOTA	163		ARG			10.301	-0.071 7.34		
	ATOM	163	9 CA	ARG	A	515	9.585	-1.327 7.56	1.00	18.05

5	ATOM	1640	CB	ARG	A	515	9.984	-1.980	8.889		18.36
	ATOM	1641	CG	ARG	Α	515	9.173	-3.237	9.213		17.84
	ATOM	1642	CD	ARG	A	515	9.823	-4.470	8.606	1.00	17.94
	ATOM	1643	NE	ARG	A	515	11.038	-4.813	9.334	1.00	26.96
	ATOM	1644	CZ	ARG	A	515	11.406	-6.051	9.641	1.00	25.13
10	MOTA	1645	NHl	ARG	Α	515	10.654	-7.080	9.281	1.00	23.49
	ATOM	1646	NH2	ARG	A	515	12.511	-6.254		1.00	32.16
	MOTA	1647	С	ARG	A	515	8.089	-1.020	7.594	1.00	18.29
	ATOM	1648	0	ARG	A	515	7.275	-1.759	7.038	1.00	16.22
	ATOM	1649	N	HIS	A	516	7.726	0.085	8.237	1.00	19.33
15	MOTA	1650	CA	HIS	A	516	6.317	0.441	8.330	1.00	17.78
	ATOM	1651	CB	HIS	A	516	6.126	1.702	9.166	1.00	16.84
	ATOM	1652	CG	HIS	Α	516	4.692	2.101	9.312	1.00	18.16
	MOTA	1653	CD2	HIS	Α	516	3.967	3.061	8.691	1.00	21.17
	MOTA	1654	ND1	HIS	A	516	3.830		10.180	1.00	20.70
20	ATOM	1655	CE1	HIS	A	516	2.633			1.00	21.52
	MOTA	1656	NE2	HIS	Α	516	2.689	2.992	9.191	1.00	20.16
	MOTA	1657	С	HIS	Α	516	5.708	0.659	6.954	1.00	16.63
	MOTA	1658	0	HIS	Α	516	4.598	0.216	6.689	1.00	18.58
	ATOM	1659	N	MET	Α	517	6.438	1.334	6.073	1.00	15.29
25	ATOM	1660	CA	MET	Α	517	5.925	1.589	4.730	1.00	16.58
	MOTA	1661	CB	MET	A	517	6.837	2.576	4.002	1.00	18.66
	MOTA	1662	CG	MET	A	517	6.805	3.978	4.631	1.00	16.88
	MOTA	1663	SD	MET	A	517	7.670	5.243	3.701	1.00	24.08
	MOTA	1664	CE	MET	A	517	9.390	4.777		1.00	14.30
30	MOTA	1665	С	MET	A	517	5.773	0.289		1.00	17.86
	ATOM	1666	0	MET	Α	517	4.791	0.101		1.00	18.25
	MOTA	1667	N	SER	A	518	6.741	-0.610		1.00	17.43
	MOTA	1668	CA	SER	A	518	6.697	-1.896		1.00	18.40
	MOTA	1669	CB	SER	A	518	7.974	-2.695		1.00	16.77
35	MOTA	1670	OG	SER	A	518	7.834	-4.030		1.00	24.23
	MOTA	1671	. C	SER	A	518	5.476	-2.695		1.00	17.91
	MOTA	1672	. 0	SER	A	518	4.788	-3.295		1.00	18.97 21.82
	MOTA	1673		ASN	A	519	5.204	-2.697		1.00	21.82
	MOTA	1674		ASN	A	519	4.047	-3.418		1.00	23.24
40	MOTA	1675		ASN	A	519	3.957	-3.257		1.00	31.14
	MOTA	1676		ASN	A	519	5.046	-4.011		1.00	32.50
	MOTA	1677		ASN	A	519	5.585	-4.999		1.00 1.00	29.10
	MOTA		ND2	ASN	A	519	5.368				
	MOTA	1679		ASN	A	519	2.761				
45	MOTA	1680		ASN	A	519	1.902				
	ATOM	1683		LYS	A	520	2.627				
	MOTA	1682		LYS	A	520	1.449				
	ATOM	1683		LYS	A	520	1.484				
	MOTA	1684		LYS	A	520	1.512				
50	MOTA	168		LYS	A	520	0.656				
	MOTA	168		LYS	A	520	-0.787				
	MOTA	168		LYS			-1.560				
	MOTA	168		LYS			1.380				
	MOTA	168		LYS			0.316				
55	MOTA	169		GLY			2.520				
	MOTA	169		GLY			2.561				
	ATOM	169		GLY			2.177				
	ATOM	169		GLY			1.426		8 -0.413		
	MOTA	169		MET			2.696				
60		169		MET			2.393				
	ATOM	169	6 CB	MET	' A	522	3.170	-5.89	8 2.042		, 23.17
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5	MOTA	1697	CG	MET.	A	522	3.396	-7.308	1.559	1.00	31.06
	ATOM	1698	SD	MET	Α	522	4.572	-7.352	0.202	1.00	34.06
	MOTA	1699	CE	MET	A	522	6.125	-7.229	1.113	1.00	29.28
	ATOM	1700	С	MET	A	522	0.893	-5.281	1.218	1.00	26.49
	ATOM	1701	0	MET	Α	522	0.268	-5.920	0.361	1.00	25.47
10	ATOM	1702	N	GLU	A	523	0.321	-4.790	2.318	1.00	24.95
10		1703	CA	GLU	A	523	-1.110	-4.954	2.566	1.00	27.15
	MOTA		CB	GLU	Ā	523	-1.555	-4.206	3.835	1.00	31.08
	MOTA	1704				523	-0.830	-4.564	5.124	1.00	38.93
	MOTA	1705	CG	GLU	A			-3.585	6.258	1.00	46.90
	MOTA	1706	CD	GLU	A	523	-1.153	-2.938	6.200	1.00	47.40
15	MOTA	1707	OE1	GLU	A	523	-2.225				
	MOTA	1708	OE2	GLU	A	523	-0.337	-3.460	7.202	1.00	47.39
	MOTA	1709	С	GLU	A	523	-1.872	-4.368	1.381	1.00	26.10
	MOTA	1710	0	GLU	A	523	-2.817	-4.964	0.882	1.00	24.25
	MOTA	1711	N	HIS	Α	524	-1.449	-3.182	0.940	1.00	24.74
20	MOTA	1712	CA	HIS	Α	524	-2.093	-2.505		1.00	26.17
	ATOM	1713	CB	HIS	A	524	-1.481		-0.379	1.00	24.64
	MOTA	1714	CG	HIS	A	524	-2.233	-0.278	-1.355	1.00	30.59
	ATOM	1715	CD2	HIS	Α	524	-3.227	0.624	-1.172	1.00	32.15
	ATOM	1716	ND1	HIS	Α	524	-2.008	-0.332	-2.713	1.00	27.46
25	MOTA	1717		HIS	A	524	-2.829	0.502	-3.326	1.00	34.58
23	MOTA	1718		HIS	A	524	-3.580		-2.413	1.00	30.50
	ATOM	1719		HIS	A	524	-1.996		-1.474	1.00	28.06
		1720		HIS	A	524	-2.976		-2.217	1.00	29.81
	MOTA			LEU	A	525	-0.811		-1.746	1.00	27.07
20	ATOM	1721		LEU	A	525	-0.594		-2.955	1.00	29.30
30	ATOM	1722			A	525	0.865		-3.051	1.00	26.39
	MOTA	1723		LEU			1.307		-4.321	1.00	29.34
	MOTA	1724		LEU	A	525			-5.562	1.00	29.61
	MOTA	1725		LEU	A	525	0.734		-4.370	1.00	29.22
~ ~	MOTA	1726		LEU	A	525	2.829			1.00	31.67
35	MOTA	1727		LEU	A	525	-1.497		-2.950		32.45
	MOTA	1728		LEU	A	525	-2.128		-3.957	1.00	
	MOTA	1729		TYR	A	526	-1.559		-1.814	1.00	36.14
	ATOM	1730		TYR	A	526	-2.397		-1.696	1.00	40.36
	MOTA	1731		TYR	A	526	-2.221		-0.324		45.27
40	MOTA	1732	2 CG	TYR	A	526	-2.849		-0.229	1.00	50.62
	MOTA	1733	CD1	TYR	A	526	-2.114		-0.537	1.00	54.55
	ATOM	1734	4 CE1	TYR	A	526	-2.698		-0.482	1.00	57.27
	MOTA	1735	5 CD2	TYR	A	526	-4.188			1.00	53.48
	MOTA	1736	6 CE2	TYR	Α	526	-4.781				55.93
45	ATOM	173	7 CZ	TYR	A	526	-4.029		0.113	1.00	56.60
	MOTA	1738	B OH	TYR	Α	526	-4.603	-13.515	-0.063		60.70
	MOTA	173	9 C	TYR	A	526	-3.852	-7.298	3 -1.893	1.00	42.83
	MOTA	174	0 0	TYR	Α	526	-4.673	-8.094	1 -2.349	1.00	43.49
	ATOM	174		SER	Α	527	-4.158	-6.05	5 -1.543	1.00	41.55
50	ATOM	174		SER	Α	527	-5.503	-5.523	3 -1.686	1.00	44.04
50	ATOM	174		SER	A	527	-5.606	-4.169	-0.979	1.00	43.47
	ATOM	174		SER	A	527	-6.954		-0.786		47.51
	ATOM	174		SER	A	527	-5.817		5 -3.172		
		174		SER	A	527	-6.883		7 -3.642		
E E	MOTA					527	-4.883		7 3.012 5 -3.901		
55	MOTA	174		MET	A				5 -5.331		
	MOTA	174		MET	A	528	-5.047		9 -5.331 9 -5.870		
	ATOM	174		MET	A	528	-3.898				
	MOTA	175		MET	A	528	-3.965		6 -5.468		
	ATOM	175		MET	A	528	-5.652		B -5.273		
60	MOTA	175		MET	Α		-5.553		4 -6.044		
	MOTA	· 175	3 C	MET	A	528	-5.087	, -5.87	1 -6.071	1.00	44.29

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5	ATOM	1754	0	MET	A	528	-5.689 -5.979 -7.137 1.00 44.02	:
	MOTA	1755	N	LYS	A	529	-4.443 -6.883 -5.499 1.00 46.78	ś
	ATOM	1756	CA	LYS	Α	529	-4.413 -8.213 -6.099 1.00 51.28	,
	ATOM	1757	CB	LYS	A	529	-3.550 -9.158 -5.261 1.00 50.87	
	MOTA	1758	CG	LYS	A	529	-2.798 -10.204 -6.071 1.00 50.55	
10	ATOM	1759	CD	LYS	A	529	-3.548 -11.520 -6.104 1.00 51.25	
	ATOM	1760	CE	LYS	A	529		
	ATOM	1761	NZ	LYS	A	529		
	ATOM	1762	C	LYS	A	529		
	ATOM	1763	0	LYS	A	529		
15	ATOM	1764	N				-6.325 -9.069 -7.266 1.00 55.50	
13	ATOM			CYS	A	530	-6.472 -8.901 -5.027 1.00 56.71	
		1765	CA	CYS	A	530	-7.833 -9.416 -4.961 1.00 58.35	;
	ATOM	1766	CB	CYS	Α	530	-8.333 -9.380 -3.517 1.00 59.78	ŀ
	MOTA	1767	SG	CYS	A	530	-7.289 -10.304 -2.358 1.00 63.19	,
•	MOTA	1768	C	CYS	A	530	-8.766 -8.609 -5.858 1.00 59.36	;
20	MOTA	1769	0	CYS	Α	530	-9.644 -9.169 -6.514 1.00 59.52	
	MOTA	1770	N	LYS	A	531	-8.569 -7.293 -5.888 1.00 59.24	
	MOTA	1771	CA	LYS	A	531	-9.390 -6.411 -6.713 1.00 60.14	
	MOTA	1772	CB	LYS	A	531	-9.158 -4.952 -6.317 1.00 58.92	
	MOTA	1773	С	LYS	A	531	-9.073 -6.615 -8.195 1.00 61.48	
25	ATOM	1774	0	LYS	A	531	-9.618 -5.928 -9.061 1.00 61.74	
	MOTA	1775	N	ASN	A	532	-8.179 -7.561 -8.474 1.00 61.65	
	ATOM	1776	CA	ASN	A	532		
	ATOM	1777	CB	aşn	A	532		
	ATOM	1778	CG	ASN	A	532		
30	ATOM	1779	OD1	ASN	A	532	-8.750 -9.985-10.878 1.00 64.66	
50	ATOM	1780	ND2	ASN	A		-8.344 -10.352-11.983 1.00 67.08	
	ATOM	1781	C C			532	-9.016 -10.836 -9.891 1.00 62.68	
	ATOM			ASN	A	532	-7.247 -6.710-10.648 1.00 59.75	
		1782	0	ASN	A	532	-7.487 -6.615-11.850 1.00 57.50)
35	MOTA	1783	N	VAL	A	533	-6.507 -5.822 -9.992 1.00 59.39	
33	ATOM	1784	CA	VAL	A	533	-5.954 -4.656-10.669 1.00 58.22	,
	MOTA	1785	CB	VAL	A	533	-6.223 -3.371 -9.865 1.00 59.20	i
	ATOM	1786	CG1	VAL	A	533	-6.181 -2.163-10.785 1.00 59.21	
	MOTA	1787	CG2	VAL	A	533	-7.574 -3.467 -9.172 1.00 59.57	,
40	ATOM	1788	C	VAL	A	533	-4.452 -4.767-10.907 1.00 57.86	;
40	MOTA	1789	0	VAL	A	533	-3.846 -3.874-11.499 1.00 60.56	
	MOTA	1790	N	VAL	A	534	-3.852 -5.863-10.451 1.00 56.03	
	ATOM	1791	CA	VAL	A	534	-2.417 -6.063-10.621 1.00 54.11	
	ATOM	1792	CB	VAL	A	534	-1.767 -6.632 -9.341 1.00 54.02	
	ATOM	1793	CG1	VAL	A	534	-0.300 -6.950 -9.601 1.00 52.37	
45	ATOM	1794	CG2	VAL	A	534	-1.900 -5.635 -8.200 1.00 55.70	
	ATOM	1795	С	VAL	A	534	-2.089 -7.008-11.770 1.00 54.31	
	ATOM	1796	0	VAL	A	534		
	ATOM	1797	N	PRO	A	535		
	ATOM	1798	CD	PRO	A	535		
50	MOTA	1799	CA	PRO	Ā	535		
-	ATOM	1800	CB				-0.949 -7.373-13.893 1.00 53.24	
	ATOM			PRO	A	535	0.011 -6.500-14.697 1.00 52.71	
		1801	CG	PRO	A	535	-0.353 -5.102-14.319 1.00 53.19	
	ATOM	1802	C	PRO	A	535	-0.296 -8.664-13.411 1.00 54.25	
5 6	ATOM	1803	0	PRO	A	535	0.121 -8.768-12.254 1.00 54.56	
55	ATOM	1804	N	LEU	A	536	-0.203 -9.645-14.299 1.00 53.63	
	MOTA	1805	CA	LEU	A	536	0.382 -10.926-13.937 1.00 53.11	
	ATOM	1806	CB	LEU	A	536	-0.250 -12.046-14.763 1.00 51.88	
	ATOM	1807	CG	LEU	A	536	-0.686 -13.256~13.938 1.00 51.83	
	MOTA	1808	CD1	LEU	A	536	-1.953 -12.917-13.173 1.00 49.51	
60	ATOM	1809	CD2	LEU	A	536	-0.905 -14.449-14.854 1.00 53.43	
	ATOM	1810	С	LEU	A	536	1.895 -10.990-14.081 1.00 52.58	
							<u></u> <u></u> <u></u> <u></u>	

								١.
5	ATOM	1811	0	LEU	A	536	2.414 -11.501-15.075 1.00 55.33	
	ATOM	1812	N	TYR	A	537	2.601 -10.462-13.087 1.00 48.72	
	ATOM	1813	CA	TYR	A	537	4.057 -10.501-13.093 1.00 44.22	
	MOTA	1814	CB	TYR	A	537	4.627 -9.134-12.709 1.00 44.52	
	ATOM	1815	CG	TYR	A	537	4.331 -8.053-13.731 1.00 45.18	
10	ATOM	1816	CD1	TYR	A	537	3.623 -6.905-13.376 1.00 43.77	
10	ATOM	1817	CE1	TYR	Α	537	3.334 -5.915-14.317 1.00 45.23	
	ATOM	1818	CD2	TYR	A	537	4.747 -8.187-15.058 1.00 46.91	
	MOTA	. 1819	CE2	TYR	A	537	4.462 -7.202-16.008 1.00 43.93	
		1820	CZ	TYR	A	537	3.757 -6.071-15.631 1.00 46.70	
1.5	ATOM		OH	TYR	A	537	3.472 -5.097-16.565 1.00 48.35	
15	ATOM	1821		TYR	A	537	4.401 -11.562-12.056 1.00 41.29	
	MOTA	1822	C		A	537	4.330 -11.319-10.856 1.00 41.82	
	MOTA	1823	0	TYR		538	4.748 -12.748-12.540 1.00 40.34	
	MOTA	1824	N	ASP	A		5.055 -13.896-11.691 1.00 38.84	
	MOTA	1825	CA	ASP	A	538	5.594 -15.037-12.554 1.00 43.47	
20	MOTA	1826	CB	ASP	A	538		
	MOTA	1827	CG	ASP	A	538		
	MOTA	1828	OD1	ASP	A	538		
	MOTA	1829	OD2	ASP	A	538		
	MOTA	1830	C	ASP	A	538	5.991 -13.676-10.508 1.00 37.28 5.620 -13.964 -9.371 1.00 38.55	
25	MOTA	1831	0	ASP	A	538		
	MOTA	1832	N	LEU	A	539	7.196 -13.200-10.766 1.00 33.83	
	MOTA	1833	CA	LEU	A	539	8.155 -12.959 -9.692 1.00 32.80	
	ATOM	1834	CB	LEU	A	539	9.419 -12.323-10.263 1.00 32.78	
	MOTA	1835	CG	LEU	A	539	10.561 -12.031 -9.292 1.00 30.93	
30	MOTA	1836	CD1	LEU	Α	539	10.913 -13.280 -8.492 1.00 33.81	
	MOTA	1837	CD2	LEU	A	539	11.758 -11.538-10.077 1.00 25.92	
	MOTA	1838	С	LEU	Α	539	7.558 -12.050 -8.614 1.00 31.85	
	MOTA	1839	0	LEU	Α	539	7.590 -12.367 -7.423 1.00 25.63	
	MOTA	1840	N	LEU	A	540	7.011 -10.917 -9.042 1.00 32.07	
35	MOTA	1841		LEU	Α	540	6.411 -9.976 -8.111 1.00 31.03	
	ATOM	1842		LEU	A	540	5.792 -8.800 -8.861 1.00 30.56	
	ATOM	1843		LEU	A	540	5.124 -7.774 -7.945 1.00 31.12	
	ATOM	1844		LEU	Α	540	6.092 -7.357 -6.838 1.00 29.76	
	ATOM	1845		LEU	A	540	4.693 -6.572 -8.762 1.00 30.85	
40	MOTA	1846		LEU	Α	540	5.337 -10.660 -7.282 1.00 34.55	
40	ATOM	1847		LEU	A	540	5.316 -10.522 -6.063 1.00 31.60	
	ATOM	1848		LEU	Α	541	4.446 -11.388 -7.941 1.00 35.64	
	ATOM	1849		LEU	A	541	3.378 -12.101 -7.245 1.00 37.84	
	MOTA	1850		LEU	A	541	2.452 -12.771 -8.255 1.00 38.49	
45	ATOM	1851		LEU	A	541	1.244 -11.932 -8.678 1.00 39.80	
73	MOTA	1852		LEU	A		0.476 -11.476 -7.448 1.00 40.02	
	MOTA	1853		LEU	A		1.713 -10.733 -9.485 1.00 40.48	
	MOTA	1854		LEU	A		3.937 -13.147 -6.275 1.00 40.10	
		185		LEU	A		3.472 -13.254 -5.137 1.00 42.72	
50	ATOM	1856		GLU	A		4.929 -13.915 -6.723 1.00 38.45	
50				GLU	A		5.535 -14.932 -5.868 1.00 39.59	
	MOTA	185			Ā		6.738 -15.566 -6.564 1.00 41.73	
	ATOM	185		GLU			6.396 -16.327 -7.831 1.00 48.34	
	MOTA	185		GLU			6.931 -17.747 -7.819 1.00 52.57	
	ATOM	186		GLU			8.049 -17.961 -7.298 1.00 52.70	
55		186					0.015	
	MOTA	186					0.200	
	MOTA	186		GLU			3.303 =1.224 ; = 1	
	MOTA	186		GLU			3.307	
	MOTA	186	5 N	MET			0.011 20.20	
60	MOTA	186	6 CA	MET				
	ATOM	186	7 CB	MET	A	. 543	8.242 -11.408 -3.963 1.00 37.34	

5	MOTA	1868	CG	MET	A	543	9.311 -11.797 -4.953 1.00 40.59
	MOTA	1869	SD	MET	A	543	10.829 -12.223 -4.114 1.00 45.64
	ATOM	1870	CE	MET	A	543	12.014 -11.399 -5.151 1.00 42.61
	ATOM	1871	C	MET	Α	543	6.287 -12.064 -2.581 1.00 37.94
	ATOM	1872	0	MET	A	543	6.413 -12.127 -1.358 1.00 39.20
10	ATOM	1873	N	LEU	A	544	
	MOTA	1874	CA	LEU			
					A	544	4.100 -11.013 -2.408 1.00 40.91
	MOTA	1875	CB	LEU	A	544	3.087 -10.344 -3.341 1.00 39.88
	ATOM	1876	CG	LEU	A	544	1.775 -9.905 -2.688 1.00 42.70
٠, ١	MOTA	1877	CD1	LEU	A	544	2.060 -8.886 -1.586 1.00 37.35
15	MOTA	1878	CD2	LEU	A	544	0.8549.317 -3.741 1.00 38.47
	ATOM	1879	С	LEU	Α	544	3.420 -12.120 -1.614 1.00 42.83
	ATOM	1880	0	LEU	Α	544	2.957 -11.899 -0.496 1.00 42.73
	MOTA	1881	N	ASP	A	545	3.367 -13.313 -2.197 1.00 46.32
	MOTA	1882	CA	ASP	A	545	2.746 -14.456 -1.539 1.00 50.65
20	MOTA	1883	CB	ASP	A	545	2.606 -15.617 -2.524 1.00 53.67
	ATOM	1884	CG	ASP	·A	545	1.703 -15.278 -3.691 1.00 57.35
	MOTA	1885	OD1	ASP	A	545	0.697 -14.568 -3.475 1.00 59.99
	ATOM	1886	OD2	ASP	A	545	1.999 -15.718 -4.824 1.00 59.68
	MOTA	1887	C	ASP	A	545	3.559 -14.898 -0.327 1.00 50.74
25	ATOM	1888	0	ASP	A	545	
	ATOM	1889	N	ALA	A	546	
	MOTA	1890	CA	ALA	A	546	
	MOTA			ALA			5.750 -15.095 0.702 1.00 53.12
		1891	CB		A	546	7.180 -14.678 0.395 1.00 53.19
30	ATOM	1892	C	ALA	A	546	5.269 -14.424 1.987 1.00 54.67
30	MOTA	1893	0	ALA	A	546	5.476 -14.940 3.085 1.00 52.32
	MOTA	1894	N	HIS	A	547	4.622 -13.270 1.838 1.00 56.66
	ATOM	1895	CA	HIS	A	547	4.102 -12.520 2.978 1.00 59.19
	MOTA	1896	CB	HIS	A	547	4.144 -11.017 2.684 1.00 56.70
	MOTA	1897	CG	HIS	A	547	5.489 -10.394 2.896 1.00 54.64
35	MOTA	1898	CD2	HIS	Α	547	6.644 -10.506 2.199 1.00 53.92
	MOTA	1899	ND1	HIS	A	547	5.748 -9.514 3.925 1.00 52.17
	ATOM	1900	CE1	HIS	A	547	7.004 -9.111 3.853 1.00 52.16
	MOTA	1901	NE2	HIS	Α	547	7.570 -9.698 2.814 1.00 51.90
	MOTA	1902	С	HIS	A	547	2.668 -12.940 3.306 1.00 62.77
40	ATOM	1903	0	HIS	A	547	1.842 -12.120 3.707 1.00 63.24
	ATOM	1904	N	ARG	A	548	2.381 -14.224 3.133 1.00 68.37
	ATOM	1905	CA	ARG	A	548	1.053 -14.758 3.411 1.00 72.75
	MOTA	1906	CB	ARG	A	548	0.243 -14.864 2.113 1.00 73.73
	MOTA	1907	CG	ARG	A	548	-1.149 -14.243 2.186 1.00 74.04
45	ATOM	1908	CD	ARG	A	548	-1.081 -12.728 2.297 1.00 74.50
	ATOM	1909	NE	ARG	A	548	-2.305 -12.167 2.863 1.00 75.04
	MOTA	1910	CZ	ARG	A	548	
	ATOM	1911	NH1	ARG			
					A	548	-1.506 -10.006 2.919 1.00 75.79
50	ATOM	1912	NH2	ARG	A	548	-3.627 -10.464 3.662 1.00 76.00
50	MOTA	1913	C	ARG	A	548	1.179 -16.133 4.061 1.00 74.94
	ATOM	1914	0	ARG	A	548	0.197 -16.697 4.549 1.00 75.15
	MOTA	1915	И	LEU	A	549	2.398 -16.665 4.063 1.00 76.49
	ATOM	1916	CA	LEU	A	549	2.669 -17.969 4.653 1.00 78.14
<i></i>	ATOM	1917	CB	LEU	A	549	2.971 -18.986 3.557 1.00 77.55
55	MOTA	1918	C	LEU	Α	549	3.846 -17.870 5.619 1.00 79.13
	MOTA	1919	0	LEU	A	549	4.892 -17.317 5.215 1.00 80.40
	ATOM	1920	OXT	LEU	Α	549	3.708 -18.341 6.769 1.00 79.46
	HETATM	1921	CP9	DES	Α	600	5.390 -3.061 -6.139 1.00 21.38
	HETATM	1922	CP8	DES	Α	600	5.834 -1.989 -5.134 1.00 22.41
60	HETATM	1923	CP7	DES	A	600	5.038 -0.714 -5.236 1.00 21.32
	HETATM	1924	CP6	DES	A	600	3.587 -0.864 -5.062 1.00 25.87
						-	2.22. 2.002 2.002 2.00

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				-20	. 6	00	2.987	-0.978 -3.784 1.00 23.92
5	HETATM					00	1.597	-1.150 -3.684 1.00 29.77
	HETATM	1926	CP2			00	0.842	-1.214 -4.871 1.00 31.40
	HETATM	1927	CP3		_	00	-0.506	-1 419 -4.824 1.00 33.36
	HETATM	1928	OP3		_	500	1.421	-1.099 -6.143 1.00 27.01
	HETATM	1929	CP4		_	500	2.793	-0.929 -6.230 1.00 27.40
10	HETATM	1930	CP5			500	5.671	0 461 -5.482 1.00 22.39
	HETATM	1931	C7		_	500	7.113	0.561 -5.809 1.00 21.75
	HETATM	1932	C6		-	500 500	7.541	0.306 -7.131 1.00 19.97
	HETATM	1933	C5	DES	-	600	8.889	0.429 -7.477 1.00 23.81
	HETATM	1934	C4	DES	_	600 600	9.814	0.804 -6.488 1.00 21.88
15	HETATM	1935	C3	DES		600 600	11.125	0.901 -6.839 1.00 22.32
	HETATM	1936	03	DES			9.423	1.066 -5.161 1.00 19.74
	HETATM	1937	C2	DES		600	8.066	0.937 -4.838 1.00 21.25
	HETATM	1938		DES	A	600	4.894	1 765 -5.443 1.00 21.47
	HETATM	1939		DES	A	600	4.959	2.468 -4.070 1.00 21.38
20	HETATM	1940		DES	A	600	14.781	-3 035-17.739 1.00 24.10
	HETATM	1941		\mathtt{CL}	A	601	12.321	21 086 25.295 1.00 64.27
	MOTA	1942		SER	В	305	12.521	22 102 27.548 1.00 64.37
	MOTA	1943	3 C	SER	В	305	13.701	22 760 27.702 1.00 66.90
	MOTA	1944	1 0	SER	В	305	12.045	23.521 25.606 1.00 63.72
25	ATOM	1945	5 N	SER	В	305	11.875	22.187 26.251 1.00 64.21
	MOTA	1946	6 CA	SER	В	305	12.193	21.293 28.484 1.00 63.09
	MOTA	194	7 N	LEU	В	306	12.133	21 133 29.757 1.00 60.98
	MOTA	194		LEU	В	306	11.884	21 200 30.913 1.00 61.23
	MOTA	194		LEU	В	306	12.221	20.417 32.183 1.00 62.23
30	MOTA	195		LEU	В	306	13.304	21 144 32.966 1.00 62.56
	MOTA	195			·B	306	10.965	20 258 33.027 1.00 64.31
	MOTA	195			В	306	13.660	\ 19 819 29.803 1.00 58.39
	MOTA	195		LEU	В	306	14.570	19 654 30.614 1.00 58.56
	MOTA	195		LEU	В	306	13.293	18 881 28.933 1.00 54.82
35	MOTA	195		ALA	В	307	13.273	17 589 28.861 1.00 50.62
	MOTA	195		ALA	В	307 307	13.092	2 16 584 28.143 1.00 51.30
	MOTA	195		ALA		307	15.303	2 17 719 28.122 1.00 46.84
	MOTA	195		ALA		307	16.196	6 16 885 28.274 1.00 45.62
	MOTA	195		ALA		307	15.43	1 18 769 27.320 1.00 43.46
4(MOTA (196		LEU		308	16.64	3 18.983 26.542 1.00 43.01
	MOTA	19			_	308	16.41	3 20 100 25.526 1.00 41.32
	MOTA	19		LEU		308	16.31	5 19.708 24.051 1.00 43.10
	MOTA	19				308	15.94	2 18.239 23.903 1.00 40.51
	MOTA	19				308	15.28	7 20.602 23.375 1.00 39.80
4	5 ATOM		65 CD			308	17.87	4 19.297 27.385 1.00 42.11
	MOTA		66 C	LEU		308	19.00	00 19.102 26.932 1.00 44.34
	MOTA		67 0	LE	-	309	17.66	59 19.775 28.608 1.00 40.66
	MOTA		68 N	SE		309	18.79	96 20.100 29.475 1.00 42.79
	MOTA		69 CF			309	18.56	52 21.447 30.163 1.00 41.25
5	MOTA 0		70 CE			309	17.45	39 21.379 31.046 1.00 46.67
	ATOM		71 00				19.07	72 19.028 30.529 1.00 42.60
	ATOM		972 C	SE			20.05	53 19.119 31.269 1.00 44.18
	MOTA		973 0	SE			18.2	17 18.012 30.596 1.00 39.44
	ATOM		974 N	LE			18.3	94 16.936 31.569 1.00 37.62
	55 ATOM	_	975 C				17.2	05 15.969 31.499 1.00 38.84
	MOTA	-	976 C				16.2	16 15.873 32.668 1.00 42.43
	MOTA	-	977 C				16.0	40 17.219 33.355 1.00 42.55
	MOTA	_	-	D1 LE			14.8	81 15.380 32.138 1.00 39.69
	OTA	-	-		EU E		19.6	91 16.174 31.285 1.00 34.11
	60 ATO	_	.980 C		EU E		_	
	ATO	м 1	.981 C	[با (EU I			
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										4.04
5	MOTA	1982	N	THR		311	20.339		•	2.34
	ATOM	1983	CA	THR	В	311	21.564			
	ATOM	1984	CB	THR	В	311	22.434	=		1.75
	MOTA	1985	OG1	THR	В	311	21.724	72.74		6.20
	ATOM	1986	CG2	THR	В	311	22.782	10.00		1.05
10	ATOM	1987	C	THR	В	311	21.145			2.37
10	MOTA	1988	Ö	THR	В	311	19.967			8.16
		1989	И	ALA	В	312	22.106			33.23
	MOTA	1990	CA	ALA	В	312	21.811			35.63
	ATOM	1990	CB	ALA	В	312	23.077	10.527 30.577		34.00
1 ~	MOTA	1991	СВ	ALA	В	312	21.210	10.489 32.240		34.29
15	MOTA			ALA	В	312	20.226	9.766 32.089		33.10
	MOTA	1993	O N	ASP	В	313	21.800	10.665 33.419		33.90
	ATOM	1994	N	ASP	В	313	21.304	9.994 34.615	1.00	34.19
	MOTA	1995	CA		В	313	22.258	10.219 35.788	1.00	42.09
	MOTA	1996	CB	ASP	В	313	23.494	9.358 35.700	1.00	44.87
20	MOTA	1997	CG	ASP	В	313	24.586	9.858 36.040	1.00	51.57
	MOTA	1998	ODl	ASP		313	23.377	8.184 35.290	1.00	46.79
	MOTA	1999	OD2	ASP	B B	313	19.925	10.520 34.971	1.00	31.99
	MOTA	2000	C	ASP		313	19.056	9.768 35.426	1.00	32.03
	MOTA	2001		ASP	В		19.733	11.819 34.763		29.38
25	MOTA	2002		GLN	В	314	18.458	12.457 35.046	1.00	29.73
	MOTA	2003		GLN	В	314	18.562	13.966 34.832	1.00	32.88
	MOTA	2004		GLN	В	314	18.970	14.732 36.085	1.00	36.47
	MOTA	2005		GLN	В	314	19.213	16.208 35.815	1.00	36.76
	MOTA	2006		GLN	В	314	19.310	16.634 34.664	1.00	38.79
30	MOTA	2007		\mathtt{GLN}	В	314	19.300		1.00	39.72
	MOTA	2008		GLN	В	314			1.00	29.11
	MOTA	2009	e C	GLN	В	314	17.409		1.00	28.82
	MOTA	2010	0	GLN	В	314	16.274		1.00	27.27
	MOTA	2013	1 N	MET	В	315	17.801		1.00	30.41
35	ATOM	2012		MET	В	315	16.900		1.00	30.10
	MOTA	201		MET	В	315	17.595		1.00	38.02
	MOTA	201	4 CG	MET	В	315	16.787		1.00	41.12
	MOTA	201	5 SD	MET	В	315	15.252		1.00	39.32
	MOTA	201		MET		315	15.890		1.00	27.99
40	MOTA	201		MET		315	16.490		1.00	26.60
	MOTA	201	8 0	MET		315	15.302		1.00	27.26
	MOTA	201	9 N	VAL	В	316	17.483			24.54
	MOTA	202	0 CA			316	17.229			26.22
	MOTA	202	1 CB			316	18.554			29.81
45	MOTA	202	2 CG			316	18.272			29.75
	MOTA	202	3 CG	2 VAI		316	19.30			27.22
	MOTA	202	4 C	IAV		316	16.32			25.55
	ATOM	202	25 0	VAI	, B		15.39			24.40
	ATOM	202		SEF	R B	317	16.60			27.63
50		202	27 CA	SEI	R B	317	15.79			31.68
50	MOTA	202		SE	R B	317	16.35			39.97
	MOTA	202		SEI	R B	317	17.49			26.73
	MOTA	203		SE	R B	317	14.34			
	MOTA	20:		SE		317	13.43	4 7.932 36.648		25.65
55		203		AL			14.13			24.19
<i>J</i> .	ATOM	20				318	12.78	6 10.049 34.969		
	ATOM	20					12.85	30 11.250 34.02		
	ATOM	20		AL			12.03	8.890 34.30		
	ATOM	20		AL			10.90	8.598 34.64		
60			37 N	LE			12.69	8.225 33.36		
O			38 C				12.09	98 7.102 32.65	2 1.00	25.42
	MOTA	۷۵					166			

5	ATOM	2039	CB	LEU	В	319	13.050	6.635 31.548		22.03
,	MOTA	2040	CG	LEU	В	319	13.264	7.622 30.394		20.71
	MOTA	2041	CD1	LEU	В	319	14.146	6.995 29.331		23.60
		2042	CD2	LEU	В	319	11.918	8.020 29.803	1.00	23.82
	ATOM		CDZ	LEU	В	319	11.729	5.926 33.564	1.00	27.26
10	MOTA	2043			В	319	10.615	5.396 33.488	1.00	28.91
10	MOTA	2044	0	LEU	В	320	12.656	5.516 34.426	1.00	26.58
	MOTA	2045	N	LEU		320	12.399	4.405 35.334	1.00	26.73
	MOTA	2046	CA	LEU	В	320	13.657	4.075 36.145	1.00	26.87
	MOTA	2047	CB	LEU	В		14.846	3.460 35.398	1.00	26.15
	MOTA	2048	CG	LEU	В	320	16.053	3.375 36.330	1.00	28.04
15	MOTA	2049	CD1	LEU	В	320	14.484	2.076 34.895	1.00	26.96
	MOTA	2050	CD2	LEU	В	320	11.249	4.722 36.290	1.00	29.19
	MOTA	2051	C	LEU	В	320	10.449	3.849 36.631	1.00	26.66
	MOTA	2052	0	LEU	В	320	11.160	5.976 36.719	1.00	29.72
	MOTA	2053	N	ASP	В	321		6.371 37.647	1.00	31.36
20	MOTA	2054		ASP	В	321	10.112	7.683 38.336	1.00	36.60
	MOTA	2055	CB	ASP	В	321	10.494		1.00	46.11
	MOTA	2056	CG	ASP	В	321	11.407 .	7.461 39.535	1.00	46.64
	MOTA	2057	OD1	ASP	В	321	10.897	7.058 40.605		45.98
	MOTA	2058	OD2	ASP	В	321	12.635	7.676 39.402	1.00	28.29
25	MOTA	2059	C	ASP	B	321	8.742	6.494 36.989	1.00	27.19
	MOTA	2060	0	ASP	В	321	7.715	6.432 37.661	1.00	28.34
	MOTA	2061	. N	ALA	В	322	8.726	6.650 35.672	1.00	25.55
	MOTA	2062	CA	ALA	В	322	7.469	6.779 34.950	1.00	23.33
	MOTA	2063	CB	ALA	В	322	7.668	7.668 33.728	1.00 1.00	22.80
30	MOTA	2064	ł C	ALA	В	322	6.911	5.420 34.523	1.00	24.54
	MOTA	2065	5 0	ALA	В	322	5.810	5.338 33.979	1.00	20.16
	MOTA	2066	5 N	GLU	В	323	7.662	4.355 34.781	1.00	21.44
	MOTA	2067	7 CA	GLU	В	323	7.229	3.021 34.386	1.00	23.72
	MOTA	2068	B CB	\mathtt{GLU}	В	323	8.196	1.982 34.938	1.00	23.58
35	MOTA	206	9 CG	GLU	В	323	9.393	1.746 34.024	1.00	25.23
	MOTA	207	0 CD	GLU	В	323	8.988	1.134 32.685	1.00	21.74
	MOTA	207	1 OE1	GLU	В	323	8.852	1.881 31.692		25.49
	MOTA	207	2 OE2	GLU	В	323	8.809	-0.095 32.624	1.00	22.35
	MOTA	207	3 C	GLU	В	323	5.796	2.696 34.810		22.34
40	MOTA	207	4 0	GLU	В	323	5.409	2.926 35.951		19.10
	MOTA	207		PRO	В	324	4.986	2.165 33.880		19.11
	MOTA	207	6 CD	PRO	В	324	5.286	1.806 32.483		
	MOTA	207	7 CA	PRO	В	324	3.607	1.839 34.242		
	MOTA	207	8 CB	PRO	В	324	2.919	1.658 32.893 1.137 32.015		
45	MOTA	207	9 CG	PRO	В	324	4.015	0.556 35.060		
	MOTA	208	0 C	PRO		324	3.619			
	MOTA	208	1 0	PRO		324	4.590	-0.200 35.028		
	MOTA	208	32 N	PRO		325	2.540	0.287 35.801 1.068 35.945		
	MOTA	208		PRO		325	1.299			
50	MOTA	208	34 CA	PRO		325	2.520	-0.940 36.603		_
	MOTA	208	35 CB	PRO		325	1.394	-0.691 37.595		_
	MOTA	208	36 CG	PRO			0.448	0.205 36.854		
	MOTA	208	37 C	PRC			2.270	-2.192 35.776		
	MOTA	208	38 0	PRC			1.853	-2.118 34.61		_
55	MOTA	208	39 N	ILE			2.538	-3.344 36.379		
	MOTA	209	90 CA	ILE			2.301			
	MOTA	209	91 CB	ILE			3.303			
	MOTA	20	92 CG:				3.011	_		
	MOTA	20	93 CG:				4.729			_
60		20	94 CD				5.241			
	MOTA	20	95 C	ILE	Е В	326	0.893	-5.020 36.14	9 1.00	, 23.63

5	ATOM	2096	0	ILE	В	326	0.632	-5.231 37.332	1.00	24.81
	MOTA	2097	N	LEU	В	327	-0.018	-5.104 35.188	1.00	19.44
	ATOM	2098	CA	LEU	В	327	-1.399	-5.437 35.493	1.00	17.03
	MOTA	2099	CB	LEU	В	327	-2.336	-4.747 34.493	1.00	18.39
	ATOM	2100	CG	LEU	В	327	-2.201	-3.216 34.373	1.00	20.69
10	MOTA	2101	CD1	LEU	В	327	-3.245	-2.679 33.406	1.00	14.87
	ATOM	2102	CD2	LEU	В	327	-2.384	-2.570 35.742	1.00	14.39
	ATOM	2103	С	LEU	В	327	-1.662	-6.928 35.499	1.00	19.87
	MOTA	2104	0	LEU	В	327	-0.854	-7.722 35.014	1.00	20.90
	MOTA	2105	N	TYR	В	328	-2.803	-7.300 36.066	1.00	20.92
15	MOTA	2106	CA	TYR	В	328	-3.202	-8.692 36.135	1.00	21.79
	MOTA	2107	CB	TYR	В	328	-3.658	-9.050 37.550	1.00	22.91
	MOTA	2108	CG	TYR	В	328	-2.515	-9.376 38.468	1.00	24.60
	MOTA	2109	CD1	TYR	В	328	-2.118	-10.696 38.677	1.00	25.93
	MOTA	2110	CEl	TYR	B	328	-1.034	-11.000 39.498	1.00	28.10
20	MOTA	2111	CD2	TYR	В	328	-1.802	-8.362 39.103	1.00	29.46
	MOTA	2112	CE2	TYR	В	328	-0.716	-8.654 39.926	1.00	35.30
	MOTA	2113	CZ	TYR	В	328	-0.338	-9.973 40.117	1.00	32.59
	ATOM	2114	OH	TYR	В	328	0.739	-10.257 40.923	1.00	37.24
	MOTA	2115	С	TYR	В	328	-4.336	-8.944 35.168	1.00	22.25
25	MOTA	2116	0	TYR	В	328	-5.115	-8.039 34.849	1.00	19.77
	MOTA	2117	N	SER	В	329	-4.420	-10.180 34.698	1.00	25.81
	MOTA	2118	CA	SER	В	329	-5.480	-10.571 33.787	1.00	29.39
	MOTA	2119	CB	SER	В	329	-5.002	-11.710 32.887	1.00	27.65
	ATOM	2120	OG	SER	В	329	-6.091	-12.329 32.233	1.00	28.98
30	MOTA	2121	С	SER	В	329	-6.625	-11.042 34.673	1.00	33.17
	MOTA	2122	0	SER	В	329	-6.453	-11.157 35.888	1.00	32.52
	ATOM	2123	N	GLU	В	330	-7.792	-11.289 34.084	1.00	38.75
	MOTA	2124	CA	GLU	В	330	-8.930	-11.776 34.859	1.00	44.91
	ATOM	2125	CB	GLU	В	330	-10.134	-11.999 33.951	1.00	45.63
35	MOTA	2126	C	GLU	В	330	-8.493	-13.093 35.491	1.00	48.62
	MOTA	2127	0	GLU	В	330	-7.739	-13.851 34.882	1.00	52.37
	MOTA	2128	N	TYR	В	331	-8.952	-13.366 36.707	1.00	51.75
	MOTA	2129	CA	TYR	В	331	-8.575	-14.596 37.396	1.00	55.25
40	MOTA	2130	CB	TYR	В	331	-8.538	-14.365 38.911	1.00	53.04
40	MOTA	2131	CG	TYR	В	331	-9.769	-13.668 39.440	1.00	50.70
	MOTA	2132	CD1	TYR	В	331	-10.880	-14.400 39.856	1.00	47.09
	MOTA	2133	CE1	TYR	В	331	-12.035	-13.762 40.292	1.00	46.43
	ATOM	2134		TYR	В	331	-9.842		1.00	47.52
	ATOM	2135	CE2	TYR	В	331		-11.625 39.913	1.00	43.98
45	MOTA	2136		TYR	В	331		-12.376 40.314	1.00	44.33
	ATOM	2137		TYR	В	331		-11.747 40.715	1.00	45.31
	ATOM	2138	С	TYR	В	331		-15.743 37.075	1.00	60.11
	MOTA	2139		TYR	В	331		-15.569 37.066	1.00	63.13
50	MOTA	2140		ASP	В	332	-8.952		1.00	61.60
50	MOTA	2141		ASP	В	332	-9.704		1.00	63.58
	MOTA	2142	CB	ASP	В	332	-10.637		1.00	65.11
	MOTA	2143	CG	ASP	В	332	-11.723		1.00	65.32
	MOTA	2144		ASP	В	332	-11.420		1.00	63.69
<i>-</i> -	ATOM	2145		ASP	В	332	-12.876		1.00	63.61
55	MOTA	2146		ASP	В	332	-8.707		1.00	62.86
	ATOM	2147		ASP	В	332	-7.853	-19.056 35.287	1.00	62.26
	MOTA	2148		PRO	В	333	-8.811		1.00	63.96
	MOTA	2149		PRO	В	333	-9.808		1.00	64.24
~ ^	MOTA	2150		PRO	В	333		-21.503 36.596	1.00	64.24
60	MOTA	2151		PRO	В	333		-22.325 37.874	1.00	64.70
	MOTA	2152	CG	PRO	В	333	-9.410	-22.071 38.347	1.00	65.00

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	WO 99/00)UU14			· ·
		_	7	222	-8.180 -22.340 35.351 1.00 63.90
5	MOTA	2133	PRO B	333	7 394 -23 214 35.007 1.00 63.70
	ATOM	2324	PRO B	333	0 303 -22 084 34.683 1.00 63.83
	MOTA	2100	THR B	334	0 649 -22 832 33.475 1.00 63.77
	ATOM	2156 CA '	THR B	334	11 065 -22 477 32.975 1.00 64.63
	ATOM		THR B		-11.065 -22.17, 55-1
10	MOTA	2158 OG1	THR B	334	-11.132 -21.076 32.07
10			THR B	334	-12.102 -22.617 54.000 - 00 62 62
	MOTA	2160 C	THR B	334	-8.634 -22.490 32.00 1 00 60 15
	MOTA	2161 0	THR B	334	-8.931 -21.774 31.150 1 00 63 14
	MOTA		ARG B	335	-7.432 -23.043 32.000 - 0 0 0 70
	MOTA		ARG B	335	-6.324 -22.620 52.020
15	MOTA		ARG B	335	-5 130 -23.007 32.00
	MOTA	2164 CB	ARG B	335	-6.667 -23.000 Sover
	MOTA	2165 C	- · ·	335	-6.302 -22.298 29.298 1.00 62.33
	MOTA	2166 0		336	-7.377 -24.194 29.884 1.00 55.25
	MOTA	2167 N		336	-7 938 -25.227 30.769 1.00 53.53
20	ATOM	2168 CD	PRO B	336	-7 698 -24.437 28.471 1.00 50.10
	MOTA	2169 CA	PRO B		_B 399 -25.799 28.476 1.00 49.70
	MOTA	2170 CB	PRO B	336	-9 164 -26.372 29.844 1.00 50.71
	MOTA	2171 CG	PRO B	336	0.602 - 23.324.27.954.1.00.44.54
	ATOM	2172 C	PRO B	336	2 202 -23 342 28 179 1.00 44.14
25	ATOM	2173 0	PRO B	336	2 207 -22 350 27 274 1.00 39.18
23	MOTA	2174 N	PHE B	337	-8.007 -22.555 - 7.00 3.00 3.8 25
	ATOM	2175 CA	PHE B	337	-8.764 -21.223 26 567 1 00 36 98
	MOTA	2176 CB	PHE B		-7.850 -20.003 20.00 a c c c c c c c c c c c c c c c c c c
	MOTA	2177 CG	PHE B		-7.229 -19.317 27.300 1 00 39 89
20		2178 CD1	PHE B		-5.846 -15.311 25.000 3 97
30	ATOM .	2179 CD2	PHE B	337	-8.023 219.002 20.005 1 00 36 85
		2180 CE1	PHE B	337	-5.262 -19.035 25.000 1 00 37 15
	MOTA	2181 CE2	PHE E	3 3 3 7	-7.449 -18.000 - 30.00 38 40
	MOTA	2182 CZ	PHE E	3 337	-6.064 -10.007 30.222 1 00 36.81
	MOTA	2182 C2 2183 C	PHE E	3 337	- q 420 - 21.333 23·2·4
35			PHE F		-8.962 -22.399 24.030 2.00 35.85
	MOTA		SER I		-10 504 -20.620 23.20
	MOTA			B 338	-11 198 -20.504 25.55
	MOTA	-		B 338	-12./13 -20.040 21.000
	MOTA	2187 CB		B 338	-13.164 -19.021 21.000
4		2188 OG		B 338	-10.761 -19.761 23.037 1.00 34.33
	MOTA	2189 C	-		-10 143 -18.855 23.591 1.00 34.32
	MOTA	2190 0	**		-11.075 -19.722 21.750 1.00 33.01
	MOTA	2191 N			-10.682 -18.579 20.950 1.00 33.54
	MOTA	2192 CA			11 146 -18.737 19.501 1.00 33.73
4	5 ATOM	2193 CB	GLU	_	-10 758 -17.553 18.623 I.00 39.11
	ATOM		GLU		10 065 -17 852 17.137 1.00 43.17
	MOTA	2195 CD	GLU	B 339	11 990 -17 785 16 600 1.00 43.20
	MOTA	2196 OE		B 339	0 924 -18 152 16.510 1.00 39.19
	ATOM			В 339	11 265 17 295 21.531 1.00 34.28
	50 ATOM		GLU	в 339	-11.265 -17.295 21.631 1.00 33.65 -10.575 -16.283 21.631 1.00 33.65
	ATOM		GLU	B 339	-10.5/5 -10.405
	MOTA	•	ALA	в 340	-12.535 -17.335 22.326 1.00 29.10
	NOTA NOTA	•	ALA	B 340	-13.194 -16.104 221-1
	ATOM			в 340	-14.696 -16.412 22.0
		•	ALA	в 340	-12.639 -15.731 23.0-0
	55 ATO	•	ALA	в 340	-12.431 -14.541 21.00
	ATO		SER	B 341	-12.407 -16.691 24.719 1.00 20.00
	ATO			B 341	-11.882 -16.386 26.044 1.00 24.20
	ATO			B 341	-11.867 -17.643 26.923 1.00 27.04
	OTA			B 34	-10.851 -18.541 26.515 1.00 33.54
	60 ATO			B 341	OO DE GAN I UU 40.2'
	OTA	M 2209 C	7,00		169
					107

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5	ATOM	2210	0	SER	В	341	-10.171	-14.82426.651	1.00	21.56
	MOTA	2211	N	MET	В	342	-9.631	-16.368 25.114	1.00	26.83
	MOTA	2212	CA	MET	В	342	-8.271	-15.865 24.954	1.00	27.24
	MOTA	2213	CB	MET	В	342	-7.477	-16.758 24.001	1.00	30.45
	MOTA	2214	CG	MET	В	342	-6.038	-16.300 23.802	1.00	35.35
10	MOTA	2215	SD	MET	В	342	-4.866	-17.667 23.777	1.00	44.57
	MOTA	2216	CE	MET	В	342	-4.034	-17.341 22.244	1.00	41.37
	MOTA	2217	С	MET	В	342	-8.322	-14.448 24.385	1.00	
	ATOM	2218	Ō	MET	В	342	-7.653	-13.541 24.874		25.31
	MOTA	2219	N	MET	В	343	-9.114	-14.278 23.345	1.00	26.67
15	ATOM	2220	CA	MET	В	343	-9.262	-12.979 22.712	1.00	25.75
	ATOM	2221	CB	MET	В	343	-10.210		1.00	25.47
	ATOM	2222	CG	MET		343		-13.088 21.528	1.00	23.51
	ATOM	2223	SD		В		-9.540	-13.618 20.273	1.00	28.86
				MET	В	343	-8.325	-12.456 19.609	1.00	29.25
20	MOTA	2224	CE	MET	В	343	-9.344	-11.015 19.371	1.00	28.74
20	ATOM	2225	C	MET	В	343	-9.798	-11.966 23.712	1.00	25.37
	ATOM	2226	0	MET	В	343	-9.360	-10.810 23.728	1.00	24.98
	ATOM	2227	N	\mathtt{GLY}	В	344	-10.739	-12.403 24.536	1.00	23.91
	MOTA	2228	CA	GLY	В	344	-11.320	-11.526 25.536	1.00	22.43
05	ATOM	2229	C	GLY	В	344	-10.313	-11.103 26.592	1.00	22.06
25	MOTA	2230	0	GLY	В	344	-10.262	-9.934 26.982	1.00	20.87
	MOTA	2231	N	LEU	В	345	-9.511	-12.048 27.063	1.00	19.36
	ATOM	2232	CA	LEU	В	345	-8.520	-11.748 28.083	1.00	25.74
	MOTA	2233	CB	LEU	В	345	-7.886	-13.040 28.600	1.00	26.78
20	MOTA	2234	CG	LEU	В	345	-8.794	-14.010 29.362	1.00	30.04
30	ATOM	2235	CD1	LEU	В	345	-8.099	-15.357 29.488	1.00	28.39
	MOTA	2236	CD2	LEU	В	345	-9.122	-13.443 30.736	1.00	29.93
	ATOM	2237	С	LEU	В	345	-7.425	-10.822 27.550	1.00	23.24
	ATOM	2238	0	LEU	В	345	-7.037	-9.865 28.212	1.00	23.43
25	ATOM	2239	N	LEU	В	346	-6.937	-11.108 26.350	1.00	21.92
35	MOTA	2240	CA	LEU	В	346	-5.874	-10.303 25.763	1.00	22.71
	ATOM	2241	CB	LEU	В	346	-5.343	-10.962 24.486	1.00	23.17
	ATOM	2242	CG	LEU	В	346	-4.684	-12.331 24.668	1.00	20.66
	ATOM	2243	CD1	LEU	В	346	-4.303	-12.916 23.309	1.00	18.75
40	ATOM	2244	CD2	LEU	В	346	-3.464	-12.188 25.553	1.00	20.84
40	MOTA	2245	C	LEU	В	346	-6.304	-8.873 25.458	1.00	22.99
	MOTA	2246	0	LEU	В	346	-5.540	-7.935 25.695	1.00	22.07
	MOTA	2247	N	THR	В	347	-7.516	-8.699 24.937	1.00	20.53
	MOTA	2248	CA	THR	В	347	-7.987	-7.357 24.608	1.00	21.89
	ATOM	2249	CB	THR	В	347	-9.152	-7.388 23.601	1.00	21.65
45	ATOM	2250	OG1	THR	В	347	-10.218	-8.190 24.123	1.00	19.65
	MOTA	2251	CG2	THR	В	347	-8.676	-7.955 22.262	1.00	22.01
	MOTA	2252	С	THR	В	347	-8.426	-6.590 25.853	1.00	23.60
	ATOM	2253	0	THR	В	347	-8.358	-5.357 25.883	1.00	20.31
	MOTA	2254	N	ASN	В	348	-8.884	-7.314 26.874	1.00	22.27
50	MOTA	2255	CA	ASN	В	348	-9.293	-6.667 28.114	1.00	23.99
	ATOM	2256	CB	ASN	В	348	-10.008	-7.642 29.056	1.00	22.32
	ATOM	2257	CG	ASN	В	348	-10.342	-7.022 30.398	1.00	28.26
	ATOM	2258	OD1	ASN	В	348	-9.478	-6.746 31.216	1.00	27.14
	ATOM	2259	ND2	ASN	В	348	-11.647	-6.764 30.625	1.00	27.14
55	ATOM	2260	C	ASN	В	348	-8.035	-6.120 28.798	1.00	19.48
	MOTA	2261	Ō	ASN	В	348	-8.014	-4.991 29.271	1.00	
	ATOM	2262	N	LEU	В	349	-6.984	-6.931 28.832		18.26
	ATOM	2263	CA	LEU	В	349	-5.724	-6.516 29.446	1.00	19.07
	ATOM	2264	CB	LEU	В	349	-4.716	-7.674 29.434	1.00	20.37
60	ATOM	2265	CG	LEU	В	349	-3.297	-7.874 29.434 -7.316 29.889	1.00	18.21
	ATOM	2266	CD1	LEU	В	349	-3.323	-6.904 31.356	1.00	18.24
					_	_ 	-3.343	~0.904 3I.356	1.00	12.44

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							-8.504 29.672 1.00 21.28
5	ATOM	2267 CD2	LEU	B 349			5 307 28 718 1.00 19.92
3	MOTA	2268 C	LEU	B 349	•	-5.131	4 322 29 349 1.00 16.56
	ATOM	2269 0	LEU	B 345		-4.738	5 391 27.391 1.00 16.67
	MOTA	2270 N	ALA	B 35	•	-5.067	4 308 26 578 1.00 17.11
	MOTA	2271 CA	ALA	B 35	-	-4.529	4 690 25 095 1.00 14.15
10	MOTA	2272 CB	ALA	B 35	-	-4.587	-2.988 26.805 1.00 17.92
10	MOTA	2273 C	ALA	B 35	•	-5.272	1 926 26 904 1.00 18.71
	MOTA	2274 0	ALA	B 35		-4.650	-3.053 26.857 1.00 17.51
	ATOM	2275 N	ASP	B 35		-6.600	-1 856 27.074 1.00 16.57
	MOTA	2276 CA	ASP	B 35		-7.409	-2 202 27.041 1.00 18.9 ⁷
15	MOTA	2277 CB	ASP	B 35		-8.902	-0.974 26.858 1.00 21.80
13	ATOM	2278 CG	ASP	_	51	-9.785	-0 292 25.824 1.00 24.62
	MOTA	2279 OD1	ASP	_	51	-9.660	-0.682 27.754 1.00 22.78
	MOTA	2280 OD2	ASP			-10.604	-1 228 28,415 1.00 16.81
	ATOM	2281 C	ASP		51	-7.064	-0.009 28.534 1.00 15.75
20	ATOM	2282 0	ASP	 -	51	-6.963	-2.056 29.438 1.00 13.97
20	MOTA	2283 N	ARG		52	-6.894	-1.509 30.742 1.00 16.09
	MOTA	2284 CA	ARG	_	52	-6.552 -6.728	2 571 31 833 1.00 15.78
	ATOM	2285 CB	ARG	_	52	-6.726 -8.189	2 919 32 189 1.00 17.93
	MOTA	2286 CG	ARG	_	52	-8.103	3.982.33.279.1.00.19.84
25	MOTA	2287 CD	ARG		352	-8.010	5 222 32 785 1.00 21.36
23	ATOM	2288 NE	ARG	_	352	-7.187	-6.075 33.387 1.00 21.18
	ATOM	2289 CZ	ARG		352	-6.579	-5.741 34.516 1.00 20.51
	MOTA	2290 NH		_	352	-6.980	-7.275 32.864 1.00 28.51
	MOTA	2291 NH			352	-5.123	3 -0.975 30.728 1.00 15.81
30		2292 C	ARG	_	352	-4.835	5 0.057 31.339 1.00 15.61
50	MOTA	2293 O	ARG		352	-4.23	1 -1.665 30.019 1.00 15.45
	MOTA	2294 N	GLU		353 353	-2.83	8 -1.228 29.935 1.00 16.59
	ATOM	2295 CA			353 353	-1.99	0 -2.243 29.168 1.00 14.64
	MOTA	2296 CE			353	-1.55	4 -3.456 29.973 1.00 18.23
3:		2297 CC			353	-0.62	0 -4.355 29.176 1.00 22.72
	MOTA	2298 CI			353 353	-1.09	9 -5.078 28.275 1.00 21.94
	MOTA	2299 O			353	0.59	9 -4.324 29.442 1.00 24.41
	MOTA		E2 GL		353	-2.72	0.119 29.219 1.00 15.85
	MOTA	2301 C	GL		353	-1.87	0.939 29.540 1.00 13.76
4	MOTA 0	2302 0	GL	_	354	-3.59	0.335 28.235 1.00 12.33
	MOTA	2303 N			354	-3.55	56 1.575 27.472 1.00 15.33
	ATOM		A LE	-	354	-4.6	16 1.534 20.500 -
	ATOM				354	-4.1	74 0.750 25.222
	MOTA	•			354	-5.3	73 0.505 22120
4	45 ATOM	•		EU B	354	-3.0	69 1.001 24.004
	MOTA			EU B	354	-3.7	47 2.805 20.302 1 00 14 28
	OTA			EU B	354	-3.1	23 3.650 20.222
	IOTA		-	AL B	355	-4.6	2.662 23.300 1 00 16.78
	OTA			AL B	355	-4.8	144 3.791 30.2.
	50 ATO			AL B	355	-5.9	325 3.427 32.02
	OTA			AL B	355	-6.0	17() 4.301 32.31
	OTA			AL B	355	-7.2	254 3.10/ 30.000 -
	ATC			AL B	355	-3.5	533 4.161 50.500 - 00 17.30
	ATC		_	AL B	355	-3.3	158 5.326 32.023
	55 ATC		_	HIS B	356	-2.	826 3.160 31.133
	ATO			HIS B	356	-1.	559 3.410 32.411 - 00 21 03
	ATO			HIS B		-1.	110 2.174 32.555 1 00 22 88
	TA			HIS B		-2.	018 1.818 34.085 1.00 22.00
	ATO			HIS B		-3.	128 1.045 34.135 1.00 21.75
	60 AT			HIS B			838 2.312 35.358 1.00 19.24
	TA	OM 2323	ND1	1110 0			
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5	ATOM	2324	CE1	HIS	В	356	-2.802	1.860 36.145	1.00	18.84
	ATOM	2325	NE2	HIS	В	356	-3.598	1.088 35.426	1.00	17.92
	ATOM	2326	С	HIS	В	356	-0.479	3.861 31.184	1.00	19.67
	MOTA	2327	0	HIS	В	356	0.424	4.614 31.547	1.00	19.61
	ATOM	2328	N	MET	В	357	-0.566	3.413 29.931	1.00	14.92
10	MOTA	2329	CA	MET	В	357	0.428	3.830 28.939	1.00	15.13
	MOTA	2330	CB	MET	В	357	0.239	3.099 27.604	1.00	13.94
	MOTA	2331	CG	MET	В	357	1.149	3.631 26.476	1.00	14.71
	ATOM	2332	SD	MET	В	357	0.747	3.014 24.826	1.00	17.75
	ATOM	2333	CE	MET	В	357	0.746	1.222 25.122	1.00	15.21
15	ATOM	2334	C	MET	В	357	0.316	5.334 28.699	1.00	14.94
•	MOTA	2335	0	MET	В	357	1.319	6.031 28.560	1.00	17.02
	ATOM	2336	N	ILE	В	358	-0.909	5.839 28.659	1.00	18.01
	ATOM	2337	CA	ILE	В	358	-1.122	7.263 28.423	1.00	19.77
	MOTA	2338	CB	ILE	В	358	-2.634	7.577 28.287	1.00	23.11
20	ATOM	2339	CG2	ILE	В	358	-2.879	9.080 28.450	1.00	25.00
	ATOM	2340	CG1	ILE	В	358	-3.137	7.105 26.913	1.00	24.19
	ATOM	2341	CD1	ILE	В	358	-4.600	6.653 26.890	1.00	20.17
	MOTA	2342	C	ILE	В	358	-0.501	8.100 29.550	1.00	22.93
	ATOM	2343	0	ILE	В	358	0.080	9.153 29.299	1.00	23.33
25	ATOM	2344	N	ASN	В	359	-0.619	7.631 30.790	1.00	22.34
	ATOM	2345	CA	ASN	В	359	-0.029	8.341 31.924	1.00	23.24
	MOTA	2346	CB	ASN	В	359	-0.480	7.726 33.224	1.00	25.10
	ATOM	2347	CG	ASN	В	359	-1.831	8.171 33.649	1.00	32.65
	MOTA	2348	OD1	ASN	В	359	-2.421	9.069 33.042	1.00	32.98
30	ATOM	2349	ND2	ASN	В	359	-2.364	7.549 34.691	1.00	33.87
30	ATOM	2350	C	ASN	В	359	1.473	8.306 31.837	1.00	24.77
	MOTA	2351	0	ASN	В	359	2.152	9.285 32.149	1.00	24.19
	MOTA	2352	N	TRP	В	360	1.995	7.149 31.438	1.00	20.82
	ATOM	2353	CA	TRP	В	360	3.439	6.965 31.310	1.00	19.29
35	ATOM	2354	CB	TRP	В	360	3.754	5.524 30.878	1.00	18.59
3.5	ATOM	2355	CG	TRP	В	360	5.085	5.363 30.176	1.00	18.21
	ATOM	2356	CD2	TRP	В	360	5.310	5.308 28.756	1.00	14.38
	ATOM	2357	CE2	TRP	В	360	6.698	5.129 28.561	1.00	13.42
	ATOM	2358	CE3	TRP	В	360	4.475	5.392 27.633	1.00	15.52
40	ATOM	2359	CD1	TRP	В	360	6.306	5.221 30.762	1.00	13.34
	ATOM	2360	NE1	TRP	В	360	7.283	5.078 29.800	1.00	16.05
	ATOM	2361	CZ2	TRP	В	360	7.272	5.032 27.288	1.00	16.84
	MOTA	2362	CZ3	TRP	В	360	5.045	5.296 26.363	1.00	15.11
	ATOM	2363	CH2	TRP	В	360	6.431	5.115 26.202	1.00	16.12
45	ATOM	2364	C	TRP	В	360	3.979	7.939 30.273	1.00	20.13
	ATOM	2365		TRP	В	360	4.991	8.606 30.497	1.00	17.26
	ATOM	2366	N	ALA	В	361	3.295	8.012 29.135	1.00	19.34
	ATOM	2367		ALA	В	361	3.708	8.900 28.051	1.00	22.01
	ATOM	2368	CB	ALA	В	361	2.682	8.855 26.921	1.00	19.53
50	MOTA	2369		ALA	В	361	3.883	10.336 28.552	1.00	22.39
50	MOTA	2370		ALA	В	361	4.858	11.005 28.210	1.00	
	MOTA	2370		LYS		362	2.932	10.794 29.361		19.57
		2371			В				1.00	21.96
	ATOM			LYS	В	362	2.966	12.139 29.923	1.00	26.45
55	MOTA	2373		LYS	В	362	1.741	12.363 30.811	1.00	29.79
33	MOTA	2374		LYS	В	362	0.426	12.417 30.064	1.00	33.57
	ATOM	2375		LYS	В	362	-0.563	13.304 30.805	1.00	36.83
	ATOM	2376		LYS	В	362	-1.620	12.490 31.512	1.00	36.89
	MOTA	2377		LYS	В	362	-2.873	13.276 31.664	1.00	39.07
60	MOTA	2378		LYS	В	362	4.223	12.379 30.757	1.00	27.77
60	ATOM	2379		LYS	В	362	4.661	13.517 30.922	1.00	26.93
	MOTA	2380	N	ARG	В	363	4.805	11.302 31.278	1.00	26.61

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			ARG	В	363	5.996 11.414 32.109 1.00 27.74
5	MOTA	2381 CA			363	5.887 10.457 33.298 1.00 28.93
	MOTA	2382 CB			363	4.650 10.704 34.158 1.00 36.07
	MOTA	2383 CG 2384 CD			363	4.569 9.745 35.344 1.00 42.83
	MOTA				363	4.477 8.344 34.928 1.00 49.79
10	MOTA		-		363	3.395 7.582 35.080 1.00 51.48
10	MOTA	2386 CZ 2387 NF			363	2.300 8.081 35.648 1.00 52.17
	ATOM	2388 NH	· ·		363	3.405 6.316 34.668 1.00 40.24 7.308 11 190 31.367 1.00 25.80
	MOTA	2389 C	ARO		363	7.308 11.130 31 00 39 36
	MOTA	2390 0	AR		363	8.3/4 11.103 21.00 24 28
15	MOTA MOTA	2391 N			364	7.231 11.005 50.000 1 00 21 87
15	MOTA	2392 C			364	8.431 10.023 1 00 21 84
	MOTA	2393 C		L B	364	8.116 10.010 1.00 1.00 1.5 95
	MOTA		G1 VA	L B	364	9.267 10.104 20.000 1 00 16 24
	MOTA		G2 VA	L B	364	7.880 0.300 20 1 00 28 14
20	MOTA	2396 C	. VA	L B	364	8.925 12.211 20 24 24
20	MOTA	2397 C) VA	T B	364	8.219 13.025 10.00 29.57
	MOTA	2398 N			365	10.141 12.551 25 1 00 20 50
	ATOM		D PF		365	11.001 11.720 100 100 100 100
	MOTA	2400	CA PI		365	10.719 13.919 29.138 1.00 32.10 12.189 13.739 29.507 1.00 32.70
25	MOTA	2401	_	RO B	365	12.170 12.671 30.545 1.00 33.35
	MOTA		_	RO B	365	10.546 14.464 27.726 1.00 32.22
	MOTA			RO B	365	11 056 13 897 26.766 1.00 37.04
	MOTA			RO B		9 821 15.570 27.609 1.00 34.09
	MOTA			LY В LY В		9 612 16 182 26.310 1.00 32.54
30	MOTA			LY B		8.241 15.969 25.700 1.00 33.46
	ATOM			LY B		7.791 16.779 24.886 1.00 33.73
	MOTA		_	HE B		7.564 14.895 26.096 1.00 31.08
	MOTA		_	HE E		6.250 14.593 25.542 1.00 28.60
2.5	ATOM			HE E		5.745 13.244 26.058 1.00 25.96 4.639 12.671 25.239 1.00 22.75
35		2411		HE E		4.629 12.071
	MOTA	2412			3 367	3.313 12.771 2. 0. 0.0 22 29
	MOTA MOTA	2414			367	4.697 12.023 1.00 25 63
	MOTA	2415		PHE I	в 367	2.2/2 12.255 21.525 1 00 20 82
40		2416		PHE 1	в 367	3.867 11.403 25.111 1 00 25 50
70	MOTA	2417			B 367	2.553
	MOTA	2418	C	PHE	в 367	5.176 15.010 20.013 37
	ATOM	2419	0		в 367	4.458 10.001 21 26
	ATOM	2420			B 368	5.049 16.143 27.009 1.00 31.20 4.020 17.151 27.277 1.00 35.71
4	5 ATOM	2421			B 368	3.817 17.412 28.795 1.00 35.98
	MOTA				B 368	2 944 16 320 29.392 1.00 37.64
	MOTA				B 368	5 157 17 495 29.508 1.00 35.81
	MOTA					4 328 18 482 26.598 1.00 35.87
	MOTA			VAL		3 450 19.330 26.457 1.00 37.71
5	MOTA 0			VAL		5 572 18 665 26.175 1.00 35.49
	ATOM			ASP		5.950 19.904 25.503 1.00 36.54
	ATOM			ASP	B 369	7.466 19.963 25.309 1.00 39.79
	MOTA			ASP ASP	B 369	8.213 20.169 26.615 1.00 44.33
	MOTA			ASP	B 369	9.409 19.807 26.684 1.00 48.45
:	55 ATOM			ASP	B 369	7.604 20.693 27.572 1.00 43.27
	MOTA			ASP	B 369	5.248 19.997 24.149 1.00 34.49
	ATON			ASP	B 369	5.131 21.074 23.571 1.00 34.51
	ATO	_		LEU	B 370	4.776 18.859 23.653 1.00 30.97
	ATOI		_	LEU	B 370	4.086 18.809 22.370 1.00 29.80
	60 ATO	-		LEU	в 370	40 200 21 700 1 110 21.41
	ATO:	7.7 7.27		-		

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5	ATOM	2438	CG	LEU	В	370	5.522	# • • • • • • • • • • • • • • • • • • •		28.07
	MOTA	2439	CD1	LEU	В	370	5.353			30.38
	MOTA	2440	CD2	LEU	В	370	6.316	17.396 20.574		22.82
	MOTA	2441	С	LEU	В	370	2.628	19.218 22.521		28.04
	MOTA	2442	0	LEU	В	370	2.066	19.151 23.611	1.00	29.71
10	MOTA	2443	N	THR	В	371	2.011	19.645 21.425	1.00	28.70
	MOTA	2444	CA	THR	В	371	0.602	20.014 21.474	1.00	30.31
	MOTA	2445	CB	THR	В	371	0.150	20.690 20.163	1.00	31.96
	MOTA	2446	OG1	THR	В	371	0.284	19.763 19.080	1.00	29.49
	MOTA	2447	CG2	THR	В	371	0.991	21.930 19.878	1.00	29.98
15	MOTA	2448	.C	THR	В	371	-0.208	18.726 21.666	1.00	30.59
	MOTA	2449	O ·	THR	В	371	0.300	17.624 21.431	1.00	27.10
	MOTA	2450	N	LEU	В	372	-1.461	18.863 22.087	1.00	27.65
	ATOM	2451	CA	LEU	В	372	-2.323	17.702 22.303	1.00	30.86
	ATOM	2452	CB	LEU	В	372	-3.722	18.147 22.737	1.00	30.11
20	ATOM	2453	CG	LEU	В	372	-4.715	17.006 22.960	1.00	32.80
	MOTA	2454	CD1	LEU	В	372	-4.231	16.147 24.126	1.00	34.10
	ATOM	2455		LEU	В	372	-6.105	17.562 23.246	1.00	31.16
	ATOM	2456		LEU	В	372	-2.437	16.863 21.034	1.00	31.77
	MOTA	2457	0	LEU	В	372	-2.417	15.629 21.078	1.00	27.06
25	ATOM	2458		HIS	В	373	-2.564	17.548 19.905	1.00	31.30
	ATOM	2459	CA	HIS	В	373	-2.685	16.888 18.614	1.00	31.35
	MOTA	2460	CB	HIS	В	373	-2.844	17.935 17.503	1.00	34.30
	MOTA	2461	. CG	HIS	В	373	-2.503	17.430 16.132	1.00	41.27
	ATOM	2462	CD2	HIS	В	373	-3.293	17.105 15.079	1.00	42.50
30	MOTA	2463	ND1	HIS	В	373	-1.205	17.220 15.715	1.00	43.69
	MOTA	2464	CE1	HIS	В	373	-1.210	16.787 14.465	1.00	48.87
	MOTA	2465	NE2	HIS	В	373	-2.465	16.708 14.056	1.00	43.72
	ATOM	2466	S C	HIS	В	373	-1.468	16.012 18.337	1.00	28.29
	MOTA	2467	7 0	HIS	В	373	-1.610	14.878 17.897	1.00	30.21
35	MOTA	2468	3 N	ASP	В	374	-0.275		1.00	28.85
	MOTA	2469	9 CA	ASP	В	374	0.950		1.00	28.28
	MOTA	2470	CB	ASP	В	374	2.178		1.00	31.33
	MOTA	247		ASP	В	374	2.433		1.00	39.07
	MOTA	247		ASP	В	374	3.195		1.00	40.60
40	MOTA	247		ASP	В	374	1.874		1.00	38.64 29.05
	MOTA	247		ASP	В	374	1.029		1.00	24.26
	MOTA		5 0	ASP	В	374	1.432		1.00	24.20
	MOTA	247		GLN	В	375	0.642			
	ATOM	247		GLN	В	375	0.667		1.00	
45	MOTA	247		GLN	В	375	0.213		1.00	
	MOTA	247		GLN	В	375	1.164		1.00	
	MOTA	248		GLN	В	375	0.623		1.00	32.82
	MOTA	248		GLN	В	375	-0.044			
50	MOTA	248			В	375	0.895			
50	ATOM	248		GLN	В	375	-0.259 0.074			
	MOTA	248		GLN	В	375		and the second s		
	MOTA	248		VAL	В	376	-1.426			
	MOTA	248		VAL	В	376	-2.409			
	ATOM	248		JAV	В	376	-3.718			
55	MOTA	248				376 376	-4.572			
	MOTA	248					-4.486			
	MOTA	249		VAL			-1.852			
	MOTA	249		VAL			-1.94			
	MOTA	249		HIS			-1.25			
60		249		HIS			-0.68	_		
	MOTA	249	4 CB	HIS	В	377	-0.07	12.300 13.000		,

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5	ATOM		CG		В	377	0.535	11.690 14.667		30.63
	MOTA	2496	CD2		В	377	1.828	11.559 14.287		31.03
	MOTA	2497	ND1	HIS	В	377	-0.217	11.086 13.683		35.05
	MOTA	2498	CE1	HIS	В	377	0.588	10.607 12.750		33.12
	MOTA	2499	NE2	HIS	В	377	1.833	10.882 13.093	1.00	31.06
10	MOTA	2500	C	HIS	В	377	0.365	10.237 17.210	1.00	24.37
	MOTA	2501	0	HIS	В	377	0.321	9.109 16.719	1.00	21.47
	MOTA	2502	N	LEU	В	378	1.307	10.609 18.072	1.00	19.24
	MOTA	2503	CA	LEU	В	378	2.365	9.691 18.474	1.00	20.09
	MOTA	2504	CB	LEU	В	378	3.363	10.402 19.388	1.00	18.64
15	MOTA	2505	CG	LEU	В	378	4.230	11.489 18.736	1.00	22.15
	MOTA	2506	CD1	LEU	В	378	5.104	12.148 19.796	1.00	22.51
	MOTA	2507	CD2	LEU	В	378	5.094	10.885 17.638	1.00	20.68
	ATOM	2508	C	LEU	В	378	1.832	8.433 19.161	1.00	18.91
	MOTA	2509	0	LEU	В	378	2.262	7.320 18.859	1.00	17.52
20	MOTA	2510	N	LEU	В	379	0.888	8.610 20.077	1.00	18.25
	MOTA	2511	CA	LEU	В	379	0.317	7.486 20.795	1.00	18.60
	MOTA	2512	CB	LEU	В	379	-0.526	7.989 21.968	1.00	16.77
	MOTA	2513	CG	LEU	В	379	0.292	8.353 23.214	1.00	17.90
	MOTA	2514	CD1	LEU	В	379	-0.578	9.092 24.211	1.00	15.84
25	MOTA	2515	CD2	LEU	В	379	0.851	7.075 23.842	1.00	22.09
	MOTA	2516	C	LEU	В	379	-0.518	6.605 19.872	1.00	20.17
	MOTA	2517	0	LEU	В	379	-0.476	5.377 19.968	1.00	18.11
	MOTA	2518	N	GLU	В	380	-1.273	7.222 18.971	1.00	19.40
	MOTA	2519	CA	GLU	В	380	-2.086	6.435 18.049	1.00	20.19
30	MOTA	2520	CB	GLU	В	380	-2.994	7.350 17.222	1.00	22.43
	MOTA	2521	CG	GLU	В	380	-4.182	7.874 18.007	1.00	25.30
	MOTA	2522	CD	GLU	В	380	-5.070	8.789 17.188	1.00	29.44
	ATOM	2523	OE1	GLU	В	380	-6.206	9.066 17.625	1.00	31.70
	MOTA	2524	OE2	GLU	В	380	-4.631	9.230 16.110	1.00	31.75
35	MOTA	2525	С	GLU	В	380	-1.210	5.594 17.117	1.00	18.92
	MOTA	2526		GLU	В	380	-1.586	4.491 16.722	1.00	19.83 17.41
	MOTA	2527		ACYS	В	381	-0.039	6.113 16.772	0.75 0.25	17.41
	ATOM	2528		BCYS	В	381	-0.035	6.113 16.779 5.384 15.887	0.25	20.19
40	MOTA	2529		ACYS	В	381	0.860 0.875	5.407 15.884	0.25	17.50
40	MOTA	2530		BCYS	В	381		6.342 15.248	0.25	24.20
	MOTA	2531		ACYS	В	381	1.870	6.406 15.226	0.25	16.63
	ATOM	2532		BCYS	В	381	1.830 1.167	7.518 14.060		33.54
	. ATOM	2533		ACYS		381 381	3.048	5.656 14.128		10.36
45	MOTA	2534		BCYS ACYS		381	1.626	4.269 16.592		20.59
45	ATOM	2535		BCYS		381	1.689	4.305 16.561		19.19
	MOTA	2536		ACYS		381	1.737	3.161 16.069		19.16
	ATOM	2537		BCYS		381	1.904	3.241 15.982		19.25
	MOTA	2538			В	382	2.134	4.560 17.785		19.04
50	ATOM	2539		ALA	В	382	2.955	3.602 18.530		20.27
50	ATOM	2540		ALA		382	4.135	4.364 19.143		18.68
	MOTA	2541		ALA	В	382	2.356	2.702 19.607		16.82
	MOTA	2542		ALA	В			1.852 20.142		13.37
	MOTA	2543		ALA	В	382	3.070 1.074			15.30
ــر حے	ATOM	2544		TRP	В	383	0.487			15.80
55	MOTA	2545		TRP	В	383		· ·		16.63
	ATOM	2546		TRP	В	383	-1.009			19.93
	MOTA	2547		TRP	В	383	-1.871			20.80
	MOTA	2548		TRP	В	383	-2.493 -3.226			19.27
~	MOTA	2549		TRP	В	383 383	-3.226 -2.506			21.32
60	MOTA	2550		TRP	В	383 383	-2.306			18.59
	MOTA	255	1 CD1	TRP	В	203	-2.236	4.314 10.933	. 1.00	10.00

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5	ATOM	2552	NEl	TRP	В	383	-3.051	1.439 18.250	1.00	23.67
	ATOM	2553	CZ2	TRP	В	383	-3.963	-0.853 18.733	1.00	21.55
	MOTA	2554	CZ3	TRP	В	383	-3.243	-1.702 20.888	1.00	20.29
	MOTA	2555	CH2	TRP	В	383	-3.960	-1.844 19.686	1.00	19.03
	ATOM	2556	C	TRP	В	383	0.701	0.579 21.020	1.00	17.35
10	ATOM	2557	0	TRP	В	383	0.982	0.010 22.077	1.00	13.92
	ATOM:	2558	N	LEU	В	384	0.568	-0.087 19.879	1.00	14.07
	MOTA	2559	CA	LEU	В	384	0.773	-1.532 19.903	1.00	15.98
	MOTA	2560	CB	LEU	В	384	0.181	-2.200 18.656	1.00	12.19
	ATOM	2561	CG	LEU	В	384	0.173	-3.735 18.720	1.00	12.97
15	ATOM	2562	CD1	LEU	В	384	-0.352	-4.240 20.089	1.00	10.65
	ATOM	2563	CD2	LEU	В	384	-0.707	-4.259 17.586		
	ATOM	2564	C	LEU	В	384	2.262		1.00	17.84
	ATOM	2565	0	LEU	В	384		-1.861 20.034	1.00	14.64
	ATOM	2566	И	GLU	В	385	2.627	-2.833 20.690	1.00	13.78
20	ATOM	2567	CA	GLU			3.116	-1.046 19.414	1.00	14.96
20	ATOM				В	385	4.565	-1.260 19.509	1.00	13.79
		2568	CB	GLU	В	385	5.336	-0.179 18.739	1.00	15.34
	ATOM	2569	CG	GLU	В	385	5.297		1.00	15.38
	ATOM	2570	CD	GLU	В	385	6.162	0.738 16.520	1.00	23.97
25	MOTA	2571	OE1	GLU	В	385	7.381	0.500 16.358	1.00	21.03
23	ATOM	2572	OE2	GLU	В	385	5.622	1.808 16.149	1.00	22.19
	MOTA MOTA	2573	C	GLU	В	385	4.963	-1.161 20.987	1.00	15.79
		2574	0	GLU	В	385	5.788	-1.942 21.463	1.00	15.04
	MOTA	2575	N	ILE	В	386	4.389	-0.213 21.690	1.00	13.32
30	ATOM	2576	CA	ILE	В	386	4.723	-0.019 23.108	1.00	14.06
50	MOTA MOTA	2577 2578	CB	ILE	В	386	4.173	1.326 23.614	1.00	15.36
	ATOM	2578	CG2	ILE	В	386	4.374	1.451 25.130	1.00	15.97
	ATOM	25 <i>19</i> 2580	CG1	ILE	В	386	4.910	2.476 22.907	1.00	17.95
	ATOM	2580	CD1 C	ILE ILE	В	386	4.118	3.768 22.874	1.00	21.12
35	ATOM	2582	0	ILE	В	386	4.227	-1.164 23.993	1.00	14.97
55	ATOM	2583	N		В	386	4.905	-1.560 24.941	1.00	19.60
	ATOM	2584	CA	LEU LEU	В	387	3.038	-1.675 23.709	1.00	15.18
	ATOM	2585	CB	LEU	B B	387	2.516	-2.791 24.478	1.00	15.98
	MOTA	2586	CG			387	1.070	-3.097 24.080	1.00	17.15
40	ATOM	2587	CD1	LEU LEU	В	387	-0.031	-2.113 24.486	1.00	19.65
40	ATOM	2588	CD1	LEU	B B	387	-1.371	-2.628 23.972	1.00	17.77
	ATOM	2589	CDZ	LEU	В	387 387	-0.075	-1.966 26.002	1.00	15.38
	ATOM	2590					3.391	-4.013 24.180		
	MOTA	2591	N O	LEU MET	В	387	3.712	-4.792 25.076		14.03
45	ATOM	2592	CA	MET	В	388	3.785	-4.178 22.921		16.43
-1.5	ATOM	2593	CB		B B	388	4.602	-5.329 22.547	1.00	16.67
	ATOM	2594	CG	MET MET		388	4.673	-5.460 21.026	1.00	14.83
	ATOM	2594			В	388	3.403	-6.066 20.453	1.00	13.91
			SD	MET	В	388	3.364	-6.193 18.675	1.00	17.23
50	MOTA	2596	CE	MET	В	388	1.906	-7.225 18.511	1.00	14.97
50	ATOM	2597	C	MET	В	388	6.004	-5.332 23.133	1.00	20.19
	MOTA	2598	0	MET	В	388	6.460	-6.366 23.636	1.00	21.50
	ATOM	2599	N	ILE	В	389	6.707	-4.203 23.074		15.34
	ATOM	2600	CA	ILE	·B	389	8.044	-4.209 23.634	1.00	15.59
55	ATOM	2601	CB	ILE	В	389	8.836	-2.911 23.322	1.00	14.95
23	MOTA	2602	CG2	ILE	В	389	8.330	-1.746 24.158	1.00	12.81
	MOTA	2603	CG1	ILE	В	389	10.325	-3.164 23.602	1.00	17.24
	ATOM	2604	CD1	ILE	В	389	11.228	-1.972 23.357	1.00	15.65
	MOTA	2605	C	ILE	В	389	7.950	-4.446 25.147	1.00	14.30
60	ATOM	2606	0	ILE	В	389	8.844	-5.044 25.739		18.72
60	MOTA	2607	N	GLY	В	390	6.855	-4.007 25.761		13.99
	MOTA	2608	CA	GLY	В	390	6.681	-4.219 27.189	1.00	14.87

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	WO 3310	00014			·
			GTV P 3	390	6.444 -5.702 27.463 1.00 18.54
5	MOTA	2609 C	-	390	6.989 -6.282 28.403 1.00 16.54
	MOTA	2610 O		391	5 623 -6.325 26.628 1.00 16.15
	MOTA	2611 N		391	5 334 -7.743 26.775 1.00 18.91
	MOTA	2612 CA		391	4.332 -8.179 25.699 1.00 19.55
	MOTA	2613 CB		391	4 157 -9 689 25.457 1.00 20.91
10	MOTA	2614 CG		391	3 580 -10 351 26.699 1.00 19.41
	MOTA	2615 CD1		391	3 232 -9.913 24.268 1.00 20.70
	MOTA	2616 CD2		391	6 649 -8 518 26 625 1.00 20.31
	ATOM	2617 C	LEU B	391	7 002 -9.352 27.465 1.00 18.66
	MOTA	2618 O	LEU B	391	7 378 -8.215 25.557 1.00 18.71
15	MOTA	2619 N	VAL B	392	9 649 -8 868 25.278 1.00 19.51
	MOTA	2620 CA	VAL B	392	9 288 -8 281 24.005 1.00 23.77
	MOTA	2621 CB	B LAV	392	10 751 -8 687 23.920 1.00 24.63
	MOTA	2622 CG1	VAL B	392	0 520 -8 773 22.767 1.00 19.94
	MOTA	2623 CG2	VAL B	392 392	9 615 -8 707 26 450 1 00 22 80
20	MOTA	2624 C	VAL B	392 392	10 336 -9.637 26.811 1.00 19.36
	MOTA	2625 O	VAL B	392	9 617 -7.522 27.046 1.00 22.10
	MOTA	2626 N	TRP B		10.492 -7.241 28.171 1.00 23.20
	MOTA	2627 CA	TRP B	393	10 388 -5 773 28.578 1.00 19.22
	MOTA	2628 CB	TRP B	393	11 056 -5 479 29.895 1.00 22.53
25	MOTA	2629 CG	TRP B	393	12 453 -5.591 30.193 1.00 20.36
	MOTA	2630 CD2		393 393	12 624 -5.208 31.545 1.00 25.65
	MOTA	2631 CE2		393 393	13 578 -5 976 29.449 1.00 22.12
	MOTA	2632 CE3		393	10 452 -5.046 31.044 1.00 23.02
	MOTA	2633 CD3		393	11 387 -4.881 32.037 1.00 24.91
30	MOTA	2634 NE		393	13 976 -5 200 32 171 1.00 23.00
	MOTA	2635 CZ		393	14.829 -5.968 30.072 1.00 23.98
	MOTA	2636 CZ		393	14.964 -5.582 31.423 1.00 23.20
	MOTA	2637 CH		393	10.208 -8.114 29.388 1.00 24.36
	MOTA	2638 C	_	393	11.128 -8.717 29.944 1.00 23.04
35	MOTA	2639 0	TRP B ARG B	394	8.952 -8.189 29.819 1.00 21.29
	MOTA	2640 N		394	8.680 -9.003 30.990 1.00 22.43
	MOTA	2641 CA	_	394	7.365 -8.601 31.667 1.00 23.97
	MOTA	2642 CB	_	394	6.259 -8.149 30.759 1.00 26.16
	MOTA	2643 CG 2644 CD		394	5.026 -7.727 31.574 1.00 20.86
40		-	_	394	3.817 - 7.937 30.786 1.00 19.54
	MOTA	20-0		394	3.327 -7.059 29.915 1.00 20.58
	MOTA			394	3.944 -5.902 29.722 1.00 17.41
	MOTA	2647 NH 2648 NH		394	2.229 -7.347 29.220 1.00 16.82
4.6	ATOM	2649 C	ARG B	394	8.695 -10.502 30.713 1.00 21.78 2.657 -11 294 31.648 1.00 23.44
45		2650 0			8.65/ -11.254 51.0
	MOTA	2651 N			8.767 -10.000
	ATOM	2652 C			8.805 -12.205
	MOTA		· · · · · · ·	_	8.200 -12.4/3 2/1000
-	MOTA	2653 C 2654 O			6.834 -14.130 2,00-
5					10.239 -12.831 23:000
	ATOM				10.458 -14.030 28.854 1.00 23.75
	ATOM				11.206 -11.938 29.210 1.00 30.79
	MOTA		A MET E		12.620 -12.307 29.205 1.00 35.07
_	ATOM		B MET E		13.479 -11.063 29.423 1.00 33.84
5	55 ATOM		G MET I		14.155 -10.569 28.171 1.00 36.66
	ATOM		•	396	15.149 -9.127 28.491 1.00 40.96
	MOTA			B 396	16.675 -9.849 28.998 1.00 39.67
	MOTA	•		в 396	12.983 -13.353 30.250 1.00 35.66
	ATON		-	B 396	13.828 -14.215 30.011 1.00 34.52
(60 ATON		-	B 397	12.348 -13.266 31.410 1.00 36.19
	OTA	4 7000 1	., 020		• 77

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5	ATOM	2666	CA	GLU	В	397	12.604 11.208 32.492 1.00 39.24
	ATOM	2667	CB	GLU	В	397	12.153 -13.605 33.821 1.00 44.38
	MOTA	2668	CG	GLU	В	397	12.983 -12.422 34.271 1.00 54.05
	MOTA	2669	CD	GLU	В	397	13.483 -12.587 35.686 1.00 56.78
	ATOM	2670	OE1	GLU	В	397	13.380 -11.621 36.470 1.00 60.90
10	ATOM	2671	OE2	GLU	В	397	13.975 -13.688 36.013 1.00 60.82
- •	MOTA	2672	C	GLU	В	397	
	ATOM	2673	0	GLU	В	397	12.021 -16.459 33.061 1.00 35.84
	MOTA	2674	N	HIS	В	398	11.100 -15.609 31.202 1.00 32.14
1.0	ATOM	2675	CA	HIS	В	398	10.347 -16.823 30.914 1.00 29.48
15	MOTA	2676	CB	HIS	В	398	8.863 -16.567 31.178 1.00 29.87
	MOTA	2677	CG	HIS	В	398	8.582 -16.111 32.574 1.00 31.80
	MOTA	2678	CD2	HIS	В	398	8.215 -16.801 33.678 1.00 29.12
	MOTA	2679	ND1	HIS	В	398	8.727 -14.799 32.972 1.00 33.27
	ATOM	2680	CE1	HIS	В	398	8.462 -14.701 34.262 1.00 32.19
20	MOTA	2681	NE2	HIS	В	398	8.148 -15.902 34.714 1.00 33.48
	MOTA	2682	C	HIS	В	398	10.556 -17.317 29.492 1.00 25.95
	MOTA	2683	0	HIS	В	398	9.637 -17.291 28.672 1.00 27.47
	ATOM	2684	N	PRO	В	399	11.771 -17.801 29.186 1.00 29.09
	MOTA	2685	CD	PRO	В	399	12.926 -17.922 30.096 1.00 29.93
25	ATOM	2686	CA	PRO	В	399	12.079 -18.300 27.845 1.00 27.40
	MOTA	2687	CB	PRO	В	399	13.434 -18.988 28.016 1.00 32.09
	ATOM	2688	CG	PRO	В	399	14.062 -18.284 29.170 1.00 30.81
	MOTA	2689	C	PRO	В	399	11.009 -19.246 27.319 1.00 29.76
	ATOM	2690	0	PRO	В	399	
30	ATOM	2691	Ň	GLY	В	400	
50	ATOM	2692	CA				
		2693	CA	GLY	В	400	9.588 -19.884 25.466 1.00 26.93
	ATOM			GLY	В	400	8.161 -19.537 25.849 1.00 26.73
	ATOM	2694	0	GLY	В	400	7.220 -20.153 25.356 1.00 28.36
25	ATOM	2695	N	LYS	В	401	7.996 -18.554 26.727 1.00 25.50
35	ATOM	2696	CA	LYS	В	401	6.668 -18.139 27.165 1.00 23.45
	ATOM	2697	CB	LYS	В	401	6.435 -18.563 28.619 1.00 28.50
	ATOM	2698	CG	LYS	В	401	6.476 -20.069 28.879 1.00 28.58
	MOTA	2699	CD	LYS	В	401	6.181 -20.353 30.349 1.00 35.47
4.0	MOTA	2700	CE	LYS	В	401	6.073 -21.847 30.635 1.00 38.59
40	MOTA	2701	NZ	LYS	В	401	7.177 -22.611 29.989 1.00 42.39
	ATOM	2702	С	LYS	В	401	6.493 -16.622 27.060 1.00 21.78
	MOTA	2703	0	LYS	В	401	7.465 -15.872 27.035 1.00 21.45
	MOTA	2704	N	LEU	В	402	5.241 -16.181 26.995 1.00 23.45
	ATOM	2705	CA	LEU	В	402	4.929 -14.759 26.925 1.00 21.37
45	MOTA	2706	CB	LEU	В	402	4.088 -14.449 25.689 1.00 18.47
	ATOM	2707	CG	LEU	В	402	4.798 -14.673 24.360 1.00 16.89
	ATOM	2708	CD1	LEU	В	402	3.821 -14.395 23.211 1.00 21.23
	MOTA	2709	CD2	LEU	В	402	6.011 -13.760 24.277 1.00 23.15
	ATOM	2710	C	LEU	В	402	4.147 -14.399 28.179 1.00 19.66
50	ATOM	2711	0	LEU	В	402	3.024 -14.880 28.381 1.00 18.05
	ATOM	2712	N	LEU	В	403	4.743 -13.559 29.019 1.00 19.54
	ATOM	2713	CA	LEU	В	403	4.099 -13.148 30.259 1.00 20.21
	ATOM	2714	CB	LEU	В	403	5.155 -12.856 31.332 1.00 23.16
	MOTA	2715	CG	LEU	В	403	4.639 -12.682 32.766 1.00 29.54
55	ATOM	2716	CD1	LEU	В	403	5.519 -13.450 33.728 1.00 32.67
- -	ATOM	2717	CD2	LEU	В	403	4.626 -11.213 33.138 1.00 32.38
	ATOM	2718	CDZ	LEU	В	403	
	ATOM	2718	0	LEU	В		3.219 -11.918 30.043 1.00 20.42
	ATOM	2719	N			403	3.638 -10.787 30.291 1.00 19.18
60				PHE	В	404	2.003 -12.145 29.565 1.00 21.44
00	ATOM	2721	CA	PHE	В	404	1.066 -11.053 29.340 1.00 21.69
	ATOM	2722	CB	PHE	В	404	-0.199 -11.598 28.687 1.00 17.26

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_		0503	aa	PHE E	3 4	104	-0.026 -11.897 27.227 1.00 19.75
5	ATOM			PHE I		404	0.364 -13.167 26.801 1.00 17.90
	MOTA				_	404	-0.210 -10.897 26.280 1.00 17.04
	MOTA	_			_	404	0.572 -13.434 25.447 1.00 19.88
	MOTA	2726	CE2	_		404	-0.007 -11.148 24.924 1.00 18.47
	MOTA	2727				404	0.386 -12.418 24.503 1.00 16.45
10	MOTA	2728	CZ	-	_	404	0.768 -10.403 30.685 1.00 21.95
	MOTA	2729	C		_	404	0.656 -9.177 30.804 1.00 22.99
	MOTA	2730	0		В	405	0.670 -11.247 31.702 1.00 21.12
	ATOM	2731	N		В	405	0.424 -10.814 33.066 1.00 22.43
	MOTA	2732	CA		В	405	-1.074 -10.603 33.304 1.00 24.69
15	MOTA	2733	CB		В	405	0.959 -11.926 33.962 1.00 22.40
	MOTA	2734	C	ALA	В	405	1.133 -13.061 33.517 1.00 21.67
	MOTA	2735	0	PRO	В	406	1.246 -11.612 35.230 1.00 25.60
	MOTA	2736	N	PRO	В	406	1.129 -10.294 35.878 1.00 23.65
	MOTA	2737	CD	PRO	В	406	1.765 -12.632 36.148 1.00 25.91
20	MOTA	2738	CA		В	406	1.899 -11.882 37.475 1.00 27.04
	ATOM	2739		PRO	В	406	2.017 -10.431 37.068 1.00 26.56
	MOTA	2740		PRO		406	0.876 -13.873 36.259 1.00 25.12
	MOTA	2741		PRO	В	406	1 368 -14.967 36.538 1.00 28.92
	MOTA	2742		PRO	В	407	-0.426 -13.713 36.039 1.00 23.53
25	MOTA	2743		ASN	В	407	-1 345 -14.852 36.109 1.00 24.09
	MOTA	2744		ASN	В	407	-2 553 -14.526 36.986 1.00 24.08
	MOTA	2745		ASN	B B	407	-3 327 -13.328 36.486 1.00 26.72
	MOTA	2746		ASN	В	407	-2 851 -12.574 35.635 1.00 22.65
	MOTA	2747		ASN	В	407	-4 528 -13.140 37.019 1.00 26.46
30	MOTA	2748		ASN	В	407	-1 820 -15.231 34.714 1.00 26.91
	MOTA	2749		asn Asn	В	407	-2.859 -15.870 34.548 1.00 28.68
	ATOM	275		LEU	В	408	-1.059 -14.816 33.708 1.00 27.28
	MOTA	275		LEU	В	408	-1.387 -15.124 32.327 1.00 27.23
	ATOM	275		LEU	В	408	-2.247 -14.030 31.699 1.00 26.61
35		275		LEU	В	408	-2.815 -14.464 30.341 1.00 27.51
	MOTA	275		LEU	В	408	-3.702 -15.692 30.546 1.00 28.75
	MOTA	275		LEU	В	408	-3.598 -13.330 29.694 1.00 25.48
	MOTA	275		LEU	В	408	-0.113 -15.316 31.514 1.00 27.56
4.0	MOTA	275		LEU	В	408	0.247 -14.465 30.695 1.00 26.86
40		275 2 7 5		LEU	В	409	0.553 -16.426 31.759 1.00 27.54
	MOTA			LEU	В	409	1.786 -16.774 31.065 1.00 31.96
	MOTA	276		LEU	В	409	2.786 -17.355 32.058 1.00 31.88
	ATOM	276 276	_	LEU	В	409	4.186 -17.703 31.562 1.00 37.72
4.7	MOTA	276			В	409	4.773 -16.551 30.770 1.00 39.57
45		276			В	409	5.066 -18.018 32.758 1.00 41.72
	MOTA	276		LEU		409	1.401 -17.805 30.009 1.00 31.53
	MOTA	. 27		LEU		409	0.921 -18.892 30.340 1.00 32.67
	MOTA	27		LEU		410	1.604 -17.465 28.746 1.00 29.58
ى م	MOTA	27		LEU		410	1.228 -18.361 27.660 1.00 31.55
5	MOTA 0	27	-	LEU			0.192 -17.672 26.762 1.00 29.83
	MOTA		70 CG	LEU			-1.047 -17.080 27.452 1.00 28.55
	MOTA					_	-1.770 -16.135 26.501 1.00 26.92
	MOTA					_	-1.979 -18.200 27.891 1.00 30.49
_	ATOM			Z DEC		_	2.397 -18.839 26.814 1.00 33.88
5	55 ATOM			LEU			3.427 -18.170 26.726 1.00 36.49
	ATOM		74 0	ASI		_	2.238 -20.013 26.206 1.00 38.80
	MOTA		75 N				3.275 -20.562 25.336 1.00 38.39
	MOTA		76 CA				3.657 -21.990 25.752 1.00 44.53
	MOTA		777 CE				2.476 -22.943 25.749 1.00 44.90
(60 ATOM	_	778 CG 779 OI				1.773 -23.035 24.719 1.00 45.70
	MOTA	1 2	779 OI) AO.			450

5	MOTA	2780	OD2	ASP	В	411	2.254 -23.603 26.786 1.00 50.54
	ATOM	2781	С	ASP	B	411	2.745 -20.551 23.909 1.00 38.57
	ATOM	2782	0	ASP	В	411	1.549 -20.341 23.686 1.00 36.48
	ATOM	2783	N	ARG	В	412	3.635 -20.777 22.949 1.00 36.85
	MOTA	2784	CA	ARG	В	412	3.259 -20.763 21.541 1.00 38.32
10	ATOM	2785	CB	ARG	В	412	4.488 -21.083 20.675 1.00 38.69
10	MOTA	2786	CG	ARG	В	. 412	4.361 -22.314 19.799 1.00 40.05
	MOTA	2787	CD	ARG	В	412	
	MOTA	2788	NE	ARG	В	412	5.540 -22.099 17.626 1.00 40.95
1.5	ATOM	2789	CZ	ARG	В	412	4.649 -22.559 16.753 1.00 41.11
15	MOTA	2790	NH1	ARG	В	412	3.777 -23.490 17.115 1.00 44.01
	MOTA	2791	NH2	ARG	В	412	4.632 -22.091 15.515 1.00 41.28
	MOTA	2792	С	ARG	В	412	2.107 -21.712 21.217 1.00 37.64
	MOTA	2793	0	ARG	В	412	1.287 -21.427 20.343 1.00 36.51
	MOTA	2794	N	ASN	В	413	2.041 -22.834 21.923 1.00 35.32
20	MOTA	2795	CA	ASN	В	413	0.974 -23.798 21.688 1.00 36.68
	MOTA	2796	CB	ASN	В	413	1.170 -25.035 22.570 1.00 37.54
	MOTA	2797	CG	ASN	В	413	2.017 -26.100 21.901 1.00 43.56
	MOTA	2798	OD1	ASN	В	413	2.309 -26.022 20.704 1.00 46.11
	MOTA	2799	ND2	ASN	В	413	2.418 -27.104 22.671 1.00 47.04
25	MOTA	2800	С	ASN	В	413	-0.383 -23.168 21.982 1.00 34.01
	MOTA	2801	0	ASN	В	413	-1.349 -23.372 21.247 1.00 32.43
	ATOM	2802	N	GLN	В	414	-0.447 -22.397 23.063 1.00 32.85
	ATOM	2803	CA	GLN	В	414	-1.685 -21.741 23.449 1.00 31.91
	ATOM	2804	CB	GLN	В	414	-1.558 -21.172 24.863 1.00 33.17
30	MOTA	2805	CG	GLN	В	414	-1.528 -22.242 25.948 1.00 32.31
	ATOM	2806	CD	GLN	В	414	-1.293 -21.667 27.327 1.00 34.63
	MOTA	2807	OE1	GLN	В	414	-0.176 -21.277 27.666 1.00 33.23
	MOTA	2808	NE2	GLN	В	414	-2.349 -21.606 28.131 1.00 34.56
	ATOM	2809	C	GLN	В	414	-2.052 -20.638 22.463 1.00 29.57
35	ATOM	2810	Ö	GLN	В.	414	-3.195 -20.204 22.409 1.00 31.32
	ATOM	2811	N	GLY	В	415	-1.077 -20.190 21.682 1.00 30.96
	ATOM	2812	CA	GLY	В	415	-1.350 -19.160 20.697 1.00 34.27
	ATOM	2813	C	GLY	В	415	-2.184 -19.725 19.562 1.00 35.27
	ATOM	2814	Ō	GLY	В	415	-2.918 -19.000 18.887 1.00 33.20
40	MOTA	2815	N	LYS	В	416	-2.070 -21.031 19.354 1.00 35.28
	MOTA	2816	CA	LYS	В	416	-2.819 -21.707 18.299 1.00 38.26
	MOTA	2817	CB	LYS	В	416	-2.398 -23.177 18.201 1.00 38.00
	ATOM	2818	CG	LYS	В	416	-0.973 -23.407 17.736 1.00 40.05
	ATOM	2819	CD	LYS	В	416	-0.405 -24.668 18.369 1.00 44.10
45	ATOM	2820		LYS	В	416	0.306 -25.541 17.346 1.00 41.85
73	MOTA	2821		LYS	В	416	
	ATOM	2822		LYS	В	416	
	ATOM	2823		LYS	В	416	
50	ATOM	2824		CYS	В	417	-4.698 -21.430 19.817 1.00 37.10
50	ATOM	2825		CYS	В	417	-6.106 -21.371 20.196 1.00 36.46
	MOTA	2826		CYS	В	417	-6.218 -21.226 21.717 1.00 39.01
	MOTA	2827		CYS	В	417	-5.674 -22.710 22.612 1.00 43.81
	ATOM	2828		CYS	В	417	-6.899 -20.277 19.491 1.00 35.19
ــر مع	ATOM	2829		CYS	В	417	-8.127 -20.296 19.485 1.00 33.92
55	MOTA	2830		VAL	В	418	-6.195 -19.316 18.906 1.00 36.04
	MOTA	2831		VAL	В	418	-6.838 -18.236 18.163 1.00 34.59
	MOTA	2832		VAL	В	418	-6.525 -16.850 18.775 1.00 34.87
	MOTA	2833		VAL	В	418	-6.831 -15.763 17.765 1.00 35.32
	ATOM	2834		VAL	В	418	-7.350 -16.630 20.036 1.00 33.65
60	MOTA	2835		VAL	В	418	-6.241 -18.317 16.764 1.00 34.17
	MOTA	2836	0	VAL	В	418	-5.020 -18.323 16.611 1.00 32.73

	110 77.5						•
£	7 mon4	2837 N	GL	U B	41	.9	-7.084 -18.388 15.740 1.00 33.44
	MOTA	2837 N 2838 CA			41		-6.554 -18.500 14.390 1.00 34.52
	ATOM	2839 CB			41		-7.681 -18.722 13.380 1.00 36.21
	MOTA	2840 CG			41		-8.597 -17.538 13.166 1.00 44.19
	MOTA	2841 CD		LU B	41		-9.4// -1/./23 11:310
10	MOTA	2841 CD 2842 OE		LU B		19	-9.157 -18.803 11.113
10	MOTA	2842 OE		LU B			-10.484 -16.993 11.813 1.00 48.91
	ATOM	2844 C		LU B		19	-5.717 -17.289 13.997 1.00 32.89
	MOTA	2845 O		LU B		19	-6.156 -16.144 14.123 1.00 31.09
	MOTA	2845 N		LY B	4	20	-4.501 -17.562 13.535 1.00 32.84
1.5	MOTA	2847 C		LY B		20	-3.594 -16.506 13.122 1.00 34.37 -3.732 -15.955 14.240 1.00 35.30
15	MOTA	2848 C		LY B	4	20	-2.722 -15.555
	MOTA MOTA	2849 0		LY B	4	20	-1.745 -15.240 25.020
	MOTA	2850 N		ET B	4	21	-3.052 -10.203 13.100
	MOTA	2851 C		ET B	4	21	-2.289 -13.780 13.325 - 00 22 54
20	MOTA	2852 C		MET B	4	121	-3.100 -13.322 1
20	MOTA	2853 C		ÆT B	4	121	-2.409 -13.270 15 11 1 1 2 2 2 40
	MOTA			MET B	. 4	121	-2.124 -13.454 40.00
	ATOM			MET B	} 4	421	-3.697 -12.000 1.000 29.67
	MOTA	2856 C		MET E		421	-0.912 -10.410 10.010
25	MOTA	2857 C) [MET E		421	0.022 -13.731 17.130
23	MOTA	2858 N	1 ,	VAL E		422	-0.766 -17.054 10.10
	ATOM			VAL E		422	0.524 -15.550 10.00 25 74
	ATOM	2860				422	0.482 -19.835 16.273 1.00 35.74 0.514 -19.992 14.753 1.00 37.64
	MOTA	2861 (422	1.659 -20.555 16.897 1.00 31.68
30	MOTA				В	422	1.669 -17.640 15.935 1.00 28.64
	MOTA		_		В	422	2 788 -17.571 16.441 1.00 26.15
	MOTA		-		B B	422 423	1 402 -17.113 14.747 1.00 28.70
	MOTA				Б В	423	2.454 -16.435 13.997 1.00 31.34
	MOTA		CA		B	423	1.963 -16.050 12.596 1.00 36.21
35	MOTA		CB CG		В	423	0.502 -16.376 12.325 1.00 45.83
	MOTA		CD		B	423	0.250 -17.865 12.144 1.00 46.71
	MOTA		OE1		В	423	-0.746 -18.368 12.706 1.00 45.97
	ATOM ATOM	2871	OE2	GLU	В	423	1.045 -10.550 -1
40		2872	C	GLU	В	423	2.928 -13.100 1 100 26 59
40	ATOM	2873	0	GLU	В	423	4.113 -14.070
	MOTA	2874	N	ILE	В	424	2.001 -14.470 43.370 -
	MOTA	2875	CA	ILE	В	424	2.381 -13.273 10.111
	MOTA	2876	CB	ILE	В	424	1.134 -12.433 20 10 20 20 21
45		2877	CG2	ILE	В	424	1.492 -11.515 1.152 1.00 29 09
•	MOTA	2878	CG1	ILE	В	424	0.564 511.017 151201 1 00 30 51
	ATOM	2879	CD1	ILE	В	424	-0.695 -11.511 15.11 1 00 24 22
	MOTA	2880	C	ILE	В	424	3.153 -13.075 17.00
	MOTA	2881	0	ILE	В	424	2 709 -14 746 18.023 1.00 21.71
5	0 ATOM	2882	N	PHE	В	425	2.700 11.720 19.223 1.00 18.85
	MOTA		CA	PHE	В	425	2 650 -16 479 19.768 1.00 22.98
	MOTA			PHE	В	425	1 EBO -16 183 20.795 1.00 22.1/
	MOTA			PHE	В	425	1 207 -17 112 21.792 1.00 25.47
	MOTA			PHE	В	425	0.843 -15 001 20.747 1.00 26.30
5	5 ATOM			PHE	В	425	0 273 -16 871 22.724 1.00 24.33
	MOTA			PHE	В	425	-0 174 -14.749 21.676 1.00 25.03
	ATOM	_		PHE	В	425 425	0 459 -15 684 22 663 1.00 26 44
	ATOM			PHE	B B	425	4.817 -15.610 18.885 1.00 20.00
	MOTA			PHE	B	425	5 741 -15.292 19.636 1.00 21.15
6	60 ATOM	_		PHE ASP	В	425	
	MOTA	1 2893	3 N	MOP	Ð		
							181 -

5	ATOM	2894	CA	ASP	В	426	6.378 -16.685 17.377 1.00 23.20
	ATOM	2895	CB	ASP	В	426	6.364 -17.510 16.090 1.00 26.53
	MOTA	2896	CG	ASP	В	426	5.992 -18.965 16.335 1.00 34.28
	ATOM	2897	OD1	ASP	В	426	6.242 -19.467 17.455 1.00 35.24
	ATOM	2898	OD2	ASP	В	426	5.448 -19.600 15.409 1.00 31.49
10	MOTA	2899	С	ASP	В	426	7.302 -15.489 17.198 1.00 21.84
	ATOM	2900	0	ASP	В	426	8.465 -15.526 17.593 1.00 21.55
	ATOM	2901	N	MET	В	427	6.788 -14.429 16.591 1.00 20.12
	ATOM	2902	CA	MET	В	427	7.597 -13.234 16.382 1.00 21.02
	ATOM	2903	CB	MET	В	427	6.836 -12.228 15.520 1.00 18.53
15	MOTA	2904	CG	MET	В	427	6.864 -12.559 14.038 1.00 27.92
	ATOM	2905	SD	MET	В	427	6.011 -11.341 13.024 1.00 32.84
	ATOM	2906	CE	MET	В	427	4.363 -11.532 13.581 1.00 33.63
	MOTA	2907	С	MET	В	427	7.945 -12.616 17.732 1.00 17.42
	MOTA	2908	0	MET	В	427	9.073 -12.180 17.950 1.00 22.09
20	ATOM	2909	N	LEU	В	428	6.968 -12.597 18.634 1.00 20.47
20	ATOM	2910	CA	LEU	В	428	7.157 -12.033 19.968 1.00 20.13
	ATOM	2911	CB	LEU	В	428	5.812 -11.964 20.706 1.00 17.58
	ATOM	2912	CG	LEU	В	428	4.852 -10.887 20.179 1.00 18.41
	ATOM	2913	CD1	LEU	В	428	3.443 -11.155 20.687 1.00 11.95
25	MOTA	2914	CD2	LEU	В	428	5.324 -9.505 20.631 1.00 17.80
25	MOTA	2915	C	LEU	В	428	8.159 -12.856 20.767 1.00 20.68
	MOTA	2916	0	LEU	В	428	9.028 -12.305 21.445 1.00 20.45
	MOTA	2917	И	LEU	B	429	8.037 -14.178 20.679 1.00 20.35
	MOTA	2918	CA	LEU	B	429	8.938 -15.082 21.382 1.00 19.82
30	MOTA	2919	CB	LEU	В	429	8.470 -16.532 21.211 1.00 23.13
50	ATOM	2920		LEU	В	429	7.189 -16.839 21.997 1.00 21.85
	MOTA	2921		LEU	В	429	6.551 -18.123 21.494 1.00 25.39
	ATOM	2922		LEU	В	429	7.537 -16.944 23.475 1.00 24.91
	ATOM	2923		LEU	В	429	10.361 -14.936 20.865 1.00 20.74
35	ATOM	2924		LEU	В	429	11.318 -14.968 21.638 1.00 21.02
33	ATOM	2925		ALA	В	430	10.495 -14.770 19.554 1.00 21.40
	ATOM	2926		ALA	В	430	11.808 -14.609 18.947 1.00 22.77
	MOTA	2927		ALA	В	430	11.677 -14.596 17.432 1.00 21.11
	MOTA	2928		ALA	В	430	12.467 -13.315 19.440 1.00 22.40
40	MOTA	2929		ALA	В	430	13.670 -13.277 19.713 1.00 20.62
10	MOTA	2930		THR	В	431	11.670 -12.258 19.567 1.00 21.09
	MOTA	2931		THR	В	431	12.183 -10.974 20.021 1.00 22.67
	ATOM	2932		THR	В	431	11.128 -9.866 19.863 1.00 23.77
	MOTA	2933		THR	В	431	10.572 -9.936 18.547 1.00 23.84
45	ATOM	2934		THR	В	431	11.762 -8.489 20.073 1.00 21.78
15	ATOM	2935		THR	В	431	12.603 -11.037 21.480 1.00 21.98
	ATOM	2936		THR	В	431	13.595 -10.429 21.879 1.00 19.85
	MOTA	2937		SER	В	432	11.844 -11.773 22.280 1.00 24.24
	ATOM	2938		SER	В	432	12.169 -11.906 23.693 1.00 26.96
50	MOTA	2939		SER	В	432	11.055 -12.661 24.423 1.00 28.00
50	MOTA	2940		SER	В	432	11.404 -12.888 25.776 1.00 30.31
	ATOM	2941		SER	В	432	13.491 -12.660 23.820 1.00 27.67
						432	14.305 -12.377 24.701 1.00 23.78
	ATOM	2942		SER	В		13.691 -13.628 22.932 1.00 29.27
55	ATOM	2943		SER	В	433	
55	ATOM	2944		SER	В	433	
	MOTA	2945		SER	В	433	
	ATOM	2946		SER	В	433	
	MOTA	2947		SER	В	433	
60	MOTA	2948		SER	В	433	
60	ATOM	2949		ARG	В	434	
	ATOM	2950	CA	ARG	В	434	16.926 -11.739 21.165 1.00 29.40

	WO SALOR	00014			;
			77G B	434	16.437 -10.912 19.977 1.00 31.56
5	MOTA	2951 CB	ARG B ARG B	434	17.428 -9.868 19.493 1.00 36.76
	MOTA	2952 CG		434	18.694 -10.502 18.919 1.00 37.76
	MOTA	2953 CD	ARG B ARG B	434	19.654 -9.479 18.516 1.00 39.50
	MOTA	2954 NE		434	20.965 -9.673 18.418 1.00 44.17
	MOTA	2955 CZ		434	21.492 -10.861 18.696 1.00 43.17
10	MOTA	2956 NH1		434	21.750 -8.671 18.048 1.00 43.05
	MOTA	2957 NH2	- -	434	17 328 -10.827 22.326 1.00 29.15
	MOTA	2958 C		434	18 515 -10.612 22.569 1.00 28.82
	MOTA	2959 0		435	16.337 -10.297 23.039 1.00 24.88
	MOTA	2960 N		435	16.600 -9.422 24.186 1.00 25.74
15	MOTA	2961 CA		435	15 278 -8.972 24.825 1.00 26.53
	MOTA	2962 CB		435	14 656 -7.758 24.183 1.00 30.94
	MOTA	2963 CG		435	15 118 -7.271 22.966 1.00 32.65
	MOTA	2964 CD1		435	13.592 -7.108 24.797 1.00 33.60
	MOTA	2965 CD2		435	14.529 -6.155 22.372 1.00 36.84
20	MOTA	2966 CE1		435	12.997 -5.989 24.208 1.00 34.96
	MOTA	2967 CE2		435	13.468 -5.516 22.995 1.00 31.64
	MOTA	2968 CZ		435	17.426 -10.184 25.233 1.00 25.39
	MOTA	2969 C		435	18 414 -9.675 25.764 1.00 22.59
	MOTA	2970 0		436	16.999 -11.405 25.528 1.00 24.58
25	MOTA	2971 N	ARG B ARG B	436	17.675 -12.253 26.503 1.00 30.25
	MOTA	2972 CA		436	16 898 -13.569 26.662 1.00 33.32
	MOTA	2973 CB		436	17 232 -14.358 27.915 1.00 38.17
	MOTA	2974 CG	ARG B ARG B	436	16 135 -15.367 28.260 1.00 37.27
	MOTA	2975 CD	ARG B	436	15 646 -16.085 27.086 1.00 43.92
30	MOTA	2976 NE	ARG B	436	14.433 -15.923 26.557 1.00 46.68
	ATOM	2977 CZ 2978 NH1		436	13 578 -15.061 27.097 1.00 45.59
	MOTA			436	14.074 -16.620 25.486 1.00 46.25
	ATOM	2979 NH2 2980 C	ARG B	436	19.110 -12.531 26.048 1.00 29.82
2.5	MOTA		ARG B	436	20.057 -12.397 26.823 1.00 28.76
35	MOTA	2981 O 2982 N	AMET B		19.269 -12.921 24.789 0.50 30.27
	ATOM	2983 N	BMET B		19.252 -12.906 24.781 0.50 31.41
	MOTA	2984 CA	AMET B		20.591 -13.212 24.253 0.50 31.98
	MOTA	2985 CA	BMET B		20.547 -13.206 24.183 0.50 33.77
40	MOTA	2986 CB	AMET E		20.489 -13.646 22.788 0.50 31.34
40	MOTA MOTA	2987 CB	BMET E	437	20.348 -13.595 22.714 0.50 35.88
	ATOM	2988 CG	AMET E	437	20.179 -15.127 22.592 0.50 33.62
	ATOM	2989 CG			21.605 -13.594 21.861 0.50 40.47
	ATOM	2990 SD		3 437	20.354 -16.099 24.109 0.50 35.21
45		2991 SD		3 437	21.247 -13.937 20.115 0.50 46.79
7.	MOTA	2992 CE		3 437	22.155 -16.194 24.259 0.50 33.20 21.837 -15.632 19.976 0.50 43.22
	MOTA	2993 CE		3 437	21.037 13.032 10.032 22 23
	MOTA	2994 C		B 437	21.496 -11.555 21.555
	ATOM	2995 C	BMET :	B 437	21.467 -12.003 21.203
50		2996 0	AMET	B 437	22.702 -12.123 21101
,ر	MOTA	2997 0	BMET	B 437	22.699 -12.102 21.102 07
	ATOM	2998 N		B 438	20.913 10.003 111111
	MOTA	2999 C	MET	B 438	21.074 3.300 1.00 29 74
	MOTA	3000 CI	_	B 438	20.930
5	5 ATOM	3001 C		B 438	21.101
ر	MOTA	3002 SI		B 438	20.425
	MOTA			B 438	21.693
	MOTA		MET	B 438	21.877
	MOTA	-	MET	B 438	22.686 -8.240 26.013 1.00 30.13 21.130 -9.721 26.646 1.00 27.14
4	MOTA 06		_	B 439	21.120
	MOTA OC			B 439	21.199 -9.359 28.038 1.00 27.34
	ATOM				

												-
5	ATOM	3008	CB	ASN	В	439		.592	-9.524 2			34.85
	ATOM	3009	CG	ASN	В	439		.624	-9.480			38.58
	ATOM	3010	OD1	ASN	В	439	21	.584	-9.620		1.00	42.99
	ATOM	3011	ND2	ASN	В	439	23	.801	-9.260		1.00	41.14
	MOTA	3012	С	ASN	В	439		.745	-7.903		1.00	26.24
10	ATOM	3013	0	ASN	В	439	21	.396	-7.106		1.00	19.76
	MOTA	3014	N	LEU	В	440	19	.625	-7.564		1.00	24.90
	MOTA	3015	CA	LEU	В	440	19	.061	-6.214		1.00	25.04
	MOTA	3016	CB	LEU	В	440	17	.761	-6.157		1.00	22.36
	MOTA	3017	CG	LEU	В	440		.087	-4.786		1.00	26.33
15	MOTA	3018	CD1	LEU	В	440	17	.958	-3.843		1.00	28.33
20	ATOM	3019	CD2	LEU	В	440	15	.704	-4.914		1.00	24.81
	ATOM	3020	С	LEU	В	440	18	.782	-5.785		1.00	24.71
	ATOM	3021	0	LEU	В	440	18	.131	-6.504		1.00	26.96
	MOTA	3022	N	GLN	В	441	19	.268	-4.609	29.452	1.00	25.54
20	MOTA	3023	CA	GLN	В	441	19	.060	-4.099	30.807	1.00	25.82
20	ATOM	3024	CB	\mathtt{GLN}	В	441	20	.250	-3.231	31.234	1.00	30.41
	MOTA	3025	CG	GLN	В	441	21	L.572	-3.956		1.00	30.50
	MOTA	3026	CD	GLN	В	441	21	1.610	-5.028	32.279	1.00	32.75
	MOTA	3027	OE1	GLN	В	441	21	Ľ.539	-4.772	33.473	1.00	36.52
25	MOTA	3028	NE2	GLN	В	441	23	1.703	-6.288		1.00	31.09
20	MOTA	3029		GLN	В	441	1.	7.789	-3.265	30.883	1.00	26.93
	MOTA	3030		GLN	В	441	1'	7.303		29.866	1.00	25.40
	MOTA	3031		GLY	В	442	1	7.266		32.096	1.00	24.56
	ATOM	3032	-	GLY	В	442	1	6.058	-2.327	32.293	1.00	22.82
30	ATOM	3033		GLY	В	442	1	6.217		31.885	1.00	24.19
50	MOTA	3034		GLY	В	442	1.	5.290	-0.279	31.341	1.00	20.21
	MOTA	3035		GLU	В	443	1	7.387		32.141	1.00	22.92
	ATOM	3036		GLU	В	443	1	7.635		31.778	1.00	23.33
	MOTA	3037		GLU	В	443	1	8.960		32.378	1.00	24.26
35	ATOM	3038		GLU	В	443	1	9.005		33.895	1.00	32.31
20	MOTA	3039		GLU	В	443	1	9.701	0.270	34.402	1.00	37.68
	ATOM	3040		GLU	В	443	1	9.343		33.948	1.00	35.23
	MOTA	3041		GLU	В	443	2	0.607		35.252	1.00	42.47
	MOTA	3042		GLU	В	443	1	7.662		30.262	1.00	23.08
40	MOTA	3043		GLU	В	443	1	7.265		29.747	1.00	21.80
	MOTA	3044		GLU	В	444	1	8.128	0.253	29.552	1.00	21.16
	ATOM	3045		GLU	В	444	1	.8.182		28.093	1.00	22.60
	ATOM	3046	6 CB	GLU	В	444	1	.9.046		27.545		
	MOTA	304		GLU	В	444	2	20.545		27.705		
45	ATOM	304		GLU	В	444	2	21.340		27.393		
	ATOM	304		GLU	В	444	2	20.817	-2.978	27.629		
	ATOM	305	0 OE2	GLU	В	444	2	22.488		26.914		
	ATOM	305		GLU	В	444	1	16.758		27.552		
	MOTA	305		GLU	В	444	3	16.377		26.597		
50	MOTA	305		PHE	В	445	=	15.987		28.176		
	MOTA	305		PHE	В	445	:	14.600		27.792		
	MOTA	305		PHE	В	445	:	13.989		7 28.675		
	MOTA	305		PHE	В	445	:	12.483		5 28.709		
	ATOM	305			В	445	:	11.746		27.575		
55		305			В	445	;	11.802		1 29.872		
22	ATOM	305						10.346	5 -2.35	9 27.592		
	MOTA	306					:	10.406		2 29.903		
	ATOM	306		PHE				9.674	4 -1.99	7 28.755		
	MOTA	306		PHE				13.758		4 27.888		
60		306		PHE				13.008		7 26.966		
	MOTA	306		VAL		446		13.87	2 1.04	4 28.986	1.00	15.90

5	ATOM	3065	CA	VAL	В	446	13.074	2.269 29.112	1.00	16.78
	ATOM	3066	CB	VAL	В	446	13.165	2.895 30.531	1.00	18.32
	ATOM	3067	CG1	VAL	В	446	12.574	1.923 31.551	1.00	21.14
	ATOM	3068	CG2	VAL	В	446	14.598	3.251 30.879	1.00	21.04
	MOTA	3069	С	VAL	В	446	13.450	3.295 28.051	1.00	17.91
10	ATOM	3070	0	VAL	В	446	12.596	4.028 27.561	1.00	19.37
	ATOM	3071	N	CYS	В	447	14.723	3.335 27.674	1.00	18.81
	MOTA	3072	CA	CYS	В	447	15.161	4.255 26.635	1.00	17.34
	ATOM	3073	CB	CYS	В	447	16.682	4.224 26.512	1.00	19.33
	ATOM	3074	SG	CYS	B	447	17.538	5.134 27.798	1.00	23.60
15	ATOM	3075	C	CYS	В	447	14.537	3.826 25.301	1.00	18.09
	ATOM	3076	ō	CYS	В	447	13.988	4.643 24.563	1.00	17.52
	ATOM	3077	N	LEU	В	448	14.623	2.533 25.006	1.00	15.60
	ATOM	3078	CA	LEU	В	448	14.072	1.994 23.767	1.00	16.67
	ATOM	3079	CB	LEU	В	448	14.328	0.490 23.684	1.00	14.82
20	ATOM	3080	CG	LEU	В	448	15.730	0.009 23.301	1.00	23.57
20	ATOM	3081	CD1	LEU	В	448	15.722	-1.522 23.169	1.00	21.61
	ATOM	3082	CD2	LEU	В	448	16.167	0.658 21.986	1.00	18.92
	ATOM	3083	C	LEU	В	448	12.573	2.249 23.652	1.00	15.98
	MOTA	3084	0	LEU	В	448	12.078	2.633 22.590	1.00	18.91
25	ATOM	3085	N	LYS	В	449	11.849	2.033 22.330	1.00	17.94
23	ATOM	3086	CA	LYS	В	449	10.405	2.232 24.733	1.00	16.66
	MOTA	3087	CB	LYS	В	449	9.796	1.745 26.047	1.00	16.45
	MOTA	3088	CG	LYS	В	449	8.285	1.861 26.115	1.00	16.12
	ATOM	3089	CD	LYS	В	449	7.730	0.952 27.193	1.00	19.09
30	ATOM	3090	CE	LYS	В	449	8.201	1.380 28.580	1.00	17.04
50	MOTA	3091	NZ	LYS	В	449	7.159	1.088 29.593	1.00	17.25
	MOTA	3092	C	LYS	В	449	10.058	3.696 24.486	1.00	18.78
	ATOM	3093	Ō	LYS	В	449	9.103	3.996 23.769	1.00	14.84
	ATOM	3094	N	SER	В	450	10.837	4.610 25.059	1.00	14.50
35	MOTA	3095	CA	SER	В	450	10.591	6.032 24.849	1.00	17.11
-	MOTA	3096	СВ	SER	В	450	11.440	6.866 25.815	1.00	21.20
	MOTA	3097		SER	В	450	10.859	6.868 27.108	1.00	30.66
	ATOM	3098	С	SER	В	450	10.921	6.418 23.405	1.00	17.84
	ATOM	3099	0	SER	В	450	10.279	7.292 22.821	1.00	18.82
40	MOTA	3100	N	ILE	В	451	11.926	5.768 22.828	1.00	16.88
	MOTA	3101	CA	ILE	В	451	12.305	6.063 21.450	1.00	17.11
	MOTA	3102	CB	ILE	В	451	13.564	5.268 21.025	1.00	16.69
	MOTA	3103		ILE	В	451	13.724	5.298 19.505	1.00	19.31
	MOTA	3104	CG1	ILE	В	451	14.804	5.897 21.676	1.00	18.96
45	MOTA	3105	CD1	ILE	В	451	16.083	5.130 21.431	1.00	18.98
	MOTA	3106	С	ILE	В	451	11.142	5.711 20.527	1.00	18.09
	ATOM	3107	0	ILE	В	451	10.820	6.464 19.608	1.00	17.07
	ATOM	3108	N	ILE	В	452	10.505	4.571 20.786	1.00	18.13
	ATOM	3109	CA	ILE	В	452	9.373	4.137 19.976	1.00	16.77
50	ATOM	3110		ILE	В	452	8.804	2.775 20.477	1.00	17.40
	MOTA	3111	CG2	ILE	В	452	7.464	2.496 19.831	1.00	14.33
	ATOM	3112	CG1	ILE	В	452	9.763	1.635 20.107	1.00	15.36
	ATOM	3113		ILE	В	452	9.449	0.323 20.805	1.00	17.76
	MOTA	3114		ILE	В	452	8.271	5.195 20.024	1.00	17.47
55	ATOM	3115		ILE	В	452	7.733	5.586 18.992	1.00	16.50
	MOTA	3116		LEU	В	453	7.943	5.665 21.222	1.00	16.06
	MOTA	3117		LEU	В	453	6.903	6.680 21.374	1.00	17.17
	ATOM	3118		LEU	В	453	6.736	7.061 22.850	1.00	16.23
	ATOM	3119		LEU	В	453	5.792	8.228 23.163	1.00	17.60
60	ATOM	3120		LEU	В	453	4.388	7.881 22.704	1.00	16.94
	ATOM	3121		LEU	В	453	5.816	8.538 24.667	1.00	17.17

5	MOTA	3122	С	LEU	В	453	7.198	7.941 20.566	1.00	19.33
	ATOM	3123	0	LEU	В	453	6.320	8.458 19.879	1.00	21.37
	MOTA	3124	N	LEU	В	454	8.434	8.428 20.636	1.00	
	ATOM	3125	CA	LEU	В	454	8.789	9.653 19.933		17.68
	ATOM	3126	CB	LEU	В	454	9.959		1.00	20.93
10	ATOM	3127		LEU	В	454		10.347 20.653	1.00	24.33
	MOTA	3128	CD1	LEU			9.735	10.699 22.130	1.00	26.16
	ATOM	3129			В	454	11.046	11.170 22.749	1.00	24.82
	ATOM		CD2	LEU	В	454	8.658	11.777 22.259	1.00	23.79
		3130		LEU	В	454	9.120	9.494 18.449	1.00	20.75
15	ATOM	3131	0 .	LEU	В	454	8.941	10.431 17.673	1.00	21.33
15	ATOM	3132	N	ASN	В	455	9.566	8.311 18.042	1.00	20.54
	ATOM	3133	CA	ASN	В	455	9.951	8.093 16.651	1.00	19.46
	MOTA	3134	CB	ASN	В	455	11.147	7.149 16.584	1.00	18.58
	MOTA	3135	CG	ASN	В	455	11.576	6.871 15.161	1.00	17.64
	MOTA	3136	OD1	ASN	В	455	12.106	7.749 14.496	1.00	18.40
20	MOTA	3137	ND2	ASN	В	455	11.343	5.648 14.686	1.00	
	ATOM	3138	C	ASN	В	455	8.925	7.580 15.655		15.06
	MOTA	3139	0	ASN	В	455	8.790	8.127 14.564	1.00	22.77
	MOTA	3140	N	SER	В	456	8.224		1.00	21.94
	MOTA	3141	CA	SER	В	456	7.260	6.514 16.023	1.00	25.90
25	MOTA	3142	CB	SER	В	456		5.873 15.135	1.00	24.76
	MOTA	3143	0G	SER	В	456	6.402	4.894 15.939	1.00	26.91
	ATOM	3144	C	SER			7.212	3.818 16.390	1.00	26.24
	ATOM	3145	0		В	456	6.385	6.774 14.272	1.00	26.52
	MOTA			SER	В	456	6.323	6.588 13 <i>.</i> 055	1.00	29.22
30	MOTA	3146	N	GLY	В	457	5.716	7.750 14.872	1.00	22.07
50	ATOM	3147	CA	GLY	В	457	4.879	8.627 14.076	1.00	25.19
		, 3148	C	GLY	В	457	5.510	9.973 13.765	1.00	28.59
	ATOM	3149	0	GLY	В	457	4.851	10.850 13.214	1.00	28.31
	ATOM	3150	N	VAL	В	458	6.789	10.130 14.092	1.00	31.65
25	ATOM	3151	CA	VAL	В	458	7.486	11.396 13.879	1.00	38.50
35	ATOM	3152	CB	$_{ m LAV}$	В	458	8.950	11.310 14.373	1.00	36.24
	MOTA	3153	CG1	VAL	В	458	9.827	10.650 13.324	1.00	38.50
	ATOM	3154	CG2	VAL	В	458	9.463	12.699 14.701	1.00	39.84
	ATOM	3155	C	VAL	В	458	7.483	11.982 12.464	1.00	46.30
	MOTA	3156	0	VAL	В	458	7.567	13.201 12.302	1.00	47.67
40	ATOM	3157	N	TYR	В	459	7.393	11.138 11.442	1.00	50.45
	ATOM	3158	CA	TYR	В	459	7.385		1.00	
	ATOM	3159	CB	TYR	В	459	8.233	10.740 9.170		57.07
,	ATOM	3160	CG	TYR	В	459	9.673		1.00	57.05
	ATOM	3161	CD1	TYR	В	459	10.284	10.680 9.611 11.786 10.203	1.00	59.29
45	MOTA	3162	CE1	TYR	В	459	11.591		1.00	60.93
	MOTA	3163	CD2	TYR	В	459		11.725 10.662	1.00	61.86
	ATOM	3164	CE2	TYR	В	459	10.414	9.510 9.486	1.00	59.46
	ATOM	3165	CZ	TYR			11.726	9.439 9.943	1.00	59.67
	ATOM	3166	OH		В	459	12.305	10.548 10.532	1.00	60.84
50	ATOM			TYR	В	459	13.593	10.477 11.009	1.00	61.39
20	ATOM	3167	C	TYR	В	459	5.976	11.753 9.514	1.00	61.22
		3168	0	TYR	В	459	5.629	12.750 8.874	1.00	62.89
	ATOM	3169	N	THR	В	460	5.166	10.730 9.768	1.00	65.15
	MOTA		CA	THR	В	460	3.783	10.702 9.309	1.00	67.76
<i>e</i>	ATOM	3171	CB	THR	В	460	3.178	9.283 9.464	1.00	68.02
55	MOTA		OG1	THR	В	460	1.890	9.235 8.836	1.00	67.03
	MOTA	3173	CG2	THR	В	460	3.040	8.916 10.938	1.00	67.31
	MOTA	3174	C	THR	В	460	2.945	11.700 10.107	1.00	70.14
	MOTA	3175	0	THR	В	460	1.715	11.641 10.099	1.00	
	ATOM	3176	N	PHE	В	461	3.625	12.620 10.788		72.35
60	MOTA		CA	PHE	В	461	2.969	13.637 11.607	1.00	72.64
	MOTA		CB	PHE	В	461	3.977	14.720 12.012	1.00	75.05
					_		3.277	14.720 12.012	1.00	75.47

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5	ATOM	3179	CG	PHE	В	461	4.235	14.789 13.492		74.32
	ATOM	3180	CD1	PHE	В	461	3.200	14.609 14.404	1.00	73.98
	ATOM	3181	CD2	PHE	В	461	5.517	15.025 13.975	1.00	75.22
	ATOM	3182	CE1	PHE	В	461	3.438	14.662 15.775	1.00	74.02
	MOTA	3183	CE2	PHE	В	461	5.765	15.080 15.344	1.00	74.50
10	ATOM	3184	CZ	PHE	В	461	4.722	14.897 16.245	1.00	74.10
	MOTA	3185	С	PHE	В	461	1.787	14.286 10.896	1.00	76.78
	MOTA	3186	0	PHE	В	461	1.775	14.279 9.645	1.00	77.08
	MOTA	3187	CB	GLU	В	470	7.873	23.789 14.718	1.00	80.19
	MOTA	3188	С	GLU	В	470	8.958	21.731 15.650	1.00	79.30
15	ATOM	3189	0	GLU	В	470	9.887	21.518 16.432	1.00	78.21
	ATOM	3190	N	GLU	В	470	9.096	22.235 13.227	1.00	80.22
	MOTA	3191	CA	GLU	В	470	9.060.	22.830 14.595	1.00	80.03
	ATOM	3192	N	GLU	В	471	7.823	21.037 15.665	1.00	78.31
	ATOM	3193	CA	GLU	В	471	7.596	19.956 16.617	1.00	75.83
20	MOTA	3194	CB	GLU	В	471	6.118	19.543 16.604	1.00	76.70
20	MOTA	3195	CG	GLU	В	471	5.742	18.544 15.516	1.00	78.42
	MOTA	3196	CD	GLU	B.	471	5.062	19.198 14.327	1.00	79.69
	ATOM	3197	OE1	GLU	В	471	3.829	19.398 14.378	1.00	80.26
	MOTA	3198	OE2	GLU	В	471	5.763	19.511 13.340	1.00	80.72
25	MOTA	3199	С	GLU	В	471	8.487	18.756 16.292	1.00	73.13
	MOTA	3200	0	GLU	В	471	8.897	18.021 17.189		73.86
	MOTA	3201	N	LYS	В	472	8.785	18.565 15.009		69.65
	MOTA	3202	CA	LYS	В	472	9.639	17.461 14.581		64.40
	ATOM	3203	CB	LYS	В	472	9.578	17.293 13.060		63.78
30	MOTA	3204	CG	LYS	В	472	8.343	16.552 12.566		64.49
	ATOM	3205	CD	LYS	В	472	8.544	16.002 11.161		63.81
	MOTA	3206	CE	LYS	В	472	7.379	16.368 10.249		64.90
	ATOM	3207	NZ	LYS	В	472	6.475	15.212 9.990		63.97
	MOTA	3208	3 C	LYS	В	472	11.071	17.749 15.014		61.03
35	MOTA	3209	9 0	LYS	В	472	11.848	16.833 15.283		60.28
	MOTA	3210	N	ASP	В	473	11.413			56.84 51.69
	MOTA	3211	L CA	ASP	В	473	12.745			50.36
	MOTA	3212		ASP	В	473	12.923			49.18
	MOTA	3213		ASP	В	473	12.923			46.85
40	MOTA	3214		ASP	В	473	13.959			
	MOTA	321	5 N	HIS	В	474	11.898			
	MOTA	321		HIS	В	474	11.923			
	MOTA	321		HIS	B	474	10.652			
	MOTA	321		HIS	В	474	10.458			
45	MOTA	321			В	474	11.095 9.510			_
	MOTA	322			В	474				
	ATOM	322			В	474	9.572 10.526			_
	MOTA	322			В	474	12.030			
	MOTA	322		HIS	В	474		and the second s		
50		322		HIS		474	12.834	_		
	MOTA		5 N	ILE		475	11.214			
	MOTA		6 CA	ILE			10.105			
	MOTA	322		ILE			10.103			
	MOTA	322					8.77			
55		322					7.59			
	MOTA	323					12.57			
	MOTA	323		ILE			13.11			
	MOTA	323		ILE			13.11			
	MOTA	323		HIS			14.42			
60			34 CA	HIS			14.42			
	MOTA	323	35 CB	HIS	з в	476	14./8	~ TJ.40# TJ.0~	,	

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5	ATOM.	3236	CG	HIS	В	476	14.132	14.781 14.486	1.00	43 64
	MOTA	3237		HIS	В	476	13.723	13.498 14.342	1.00	43.64
	ATOM	3238	ND1	HIS	В	476	13.816	15.419 13.306	1.00	45.25
	ATOM	3239	CE1	HIS	В	476	13.238	14.560 12.484		48.37
	MOTA	3240		HIS	В	476	13.170	13.387 13.089	1.00	48.87
10	MOTA	3241		HIS	В	476	15.506	15.213 18.022	1.00	48.11
	ATOM	3242		HIS	В	476	16.442	14.436 18.208	1.00	31.20
	ATOM	3243	N	ARG	В	477	15.387		1.00	27.25
	MOTA	3244		ARG	В	477	16.361	16.365 18.684	1.00	30.64
	ATOM	3245	CB	ARG	В	477	16.144	16.754 19.703	1.00	30.09
15	ATOM	3246	CG	ARG	В	477	16.322	18.214 20.121	1.00	33.46
	MOTA	3247		ARG	В	477		19.212 18.982	1.00	40.74
	ATOM	3248	NE	ARG	В	477	16.274	20.649 19.479	1.00	45.91
	ATOM	3249	CZ	ARG	В	477	17.514	21.020 20.155	1.00	51.37
	ATOM	3250	NH1	ARG	В		18.375	21.927 19.702	1.00	53.68
20	ATOM	3251	NH2	ARG	В	477	18.140	22.567 18.560	1.00	53.04
	ATOM	3252	C	ARG		477	19.480	22.185 20.389	1.00	51.79
	MOTA	3253	0	ARG	В	477	16.232	15.835 20.925	1.00	26.97
	ATOM	3254	N		В	477	17.233	15.387 21.486	1.00	27.34
	MOTA	3255		VAL	В	478	14.999	15.558 21.338	1.00	23.70
25	ATOM	3255	CA CB	VAL	В	478	14.780	14.685 22.482	1.00	24.79
	ATOM	3257	CG1	VAL	В	478	13.286	14.613 22.861	1.00	24.83
	ATOM	3258		VAL	В	478	13.088	13.646 24.022	1.00	26.23
	ATOM	3259	CG2 C	VAL	В	478	12.781	15.996 23.243	1.00	28.26
	ATOM	3260	_	VAL	В	478	15.284	13.294 22.112	1.00	26.10
30	ATOM	3260	0	VAL	В	478	15.919	12.613 22.927	1.00	24.28
50	ATOM	3261	N	LEU	В	479	15.021	12.889 20.870	1.00	22.92
	ATOM		CA	LEU	В	479	15.456	11.584 20.379	1.00	21.96
	ATOM	3263	CB	LEU	В	479	14.992	11.372 18.930	1.00	22.63
	ATOM	3264	CG	LEU	В	479	13.575	10.798 18.756	1.00	20.82
35	ATOM	3265	CD1	LEU	В	479	13.231	10.689 17.274	1.00	22.53
55	ATOM	3266	CD2	LEU	В	479	13.495	9.440 19.420	1.00	23.08
	ATOM	3267	C	LEU	В	479	16.975	11.471 20.453	1.00	21.90
	ATOM	3268	0	LEU	В	479	17.506	10.416 20.778	1.00	23.11
	ATOM	3269 3270	N	ASP	В	480	17.675	12.560 20.143	1.00	23.65
40	ATOM		CA	ASP	В	480	19.141	12.566 20.198	1.00	24.29
10	ATOM	3271	CB	ASP	В	480	19.692	13.889 19.649	1.00	26.88
	ATOM	3272	CG	ASP	В	480	19.773	13.914 18.129	1.00	33.32
	ATOM	3273	OD1	ASP	В	480	19.857	12.836 17.499	1.00	35.44
	ATOM		OD2	ASP	В	480	19.757	15.022 17.563	1.00	32.44
45	ATOM	3275	C	ASP	В	480	19.590	12.406 21.656	1.00	24.13
45	ATOM	3276	0	ASP	В	480	20.551	11.697 21.956	1.00	24.88
	ATOM	3277	N	LYS	В	481	18.887	13.077 22.560	1.00	25.18
		3278	CA	LYS	В	481	19.213	13.010 23.980	1.00	26.78
	ATOM	3279	CB	LYS	В	481	18.262	13.898 24.785	1.00	31.37
50	MOTA	3280	CG	LYS	В	481	18.962	14.788 25.804	1.00	43.84
30	ATOM	3281	CD	LYS	В	481	18.780	14.260 27.219	1.00	46.08
	ATOM	3282	CE	LYS	В	481	20.120	13.928 27.865	1.00	50.99
	MOTA	3283	NZ	LYS	В	481	21.177	14.922 27.511	1.00	54.35
	MOTA	3284	С	LYS	В	481	19.124	11.575 24.495	1.00	26.87
55	ATOM	3285	0	LYS	В	481	19.951	11.145 25.305	1.00	20.37
22	ATOM	3286	N	ILE	В	482	18.124	10.830 24.027	1.00	23.26
	ATOM	3287	CA	ILE	В	482	17.981	9.452 24.472	1.00	21.07
	MOTA	3288	CB	ILE	В	482	16.655	8.828 24.015	1.00	19.80
	ATOM	3289	CG2	ILE	В	482	16.580	7.370 24.491	1.00	17.40
60	ATOM	3290	CG1	ILE	В	482	15.479	9.606 24.602	1.00	17.16
60	ATOM	3291	CD1	ILE	В	482	14.136	9.209 23.991	1.00	19.43
	MOTA	3292	C	ILE	В	482	19.135	8.616 23.947	1.00	20.21
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4	ATOM	3293	0	ILE	В	482	19.621	7.722 24.640		25.55
5	ATOM	3294	И		В	483	19.569	8.896 22.722		21.89
	ATOM	3295	CA		В	483	20.701	8.176 22.141		22.67
	MOTA	3296	CB	THR	В	483	21.030	8.662 20.695		23.34
	ATOM	3297	OG1	THR	В	483	19.890	8.475 19.851	1.00	27.33
10	MOTA	3298	CG2	THR	В	483	22.203	7.882 20.116	1.00	24.46
10	ATOM	3299	C	THR	В	483	21.913	8.441 23.035	1.00	23.51
	MOTA	3300	Ō	THR	В	483	22.650	7.520 23.381	1.00	27.01
	ATOM	3301	N	ASP	В	484	22.119	9.703 23.404	1.00	22.88
	MOTA	3302	CA	ASP	В	484	23.237	10.058 24.276	1.00	24.93
15	MOTA	3303	CB	ASP	В	484	23.201	11.546 24.652	1.00	28.69
13	MOTA	3304	CG	ASP	В	484	23.504	12.464 23.485	1.00	29.19
	MOTA	3305	OD1	ASP	В	484	23.982	11.984 22.437	1.00	29.63
	MOTA	3306	OD2	ASP	В	484	23.256	13.681 23.627	1.00	32.02
	ATOM	3307	С	ASP	В	484	23.125	9.249 25.567	1.00	24.40
20	MOTA	3308	0	ASP	В	484	24.125	8.780 26.103	1.00	25.60
20	MOTA	3309		THR	В	485	21.899	9.096 26.066	1.00	20.16
	MOTA	3310		THR	В	485	21.670	8.365 27.307	1.00	22.28
	ATOM	3311		THR	В	485	20.203	8.521 27.763	1.00	24.64
	MOTA	3312		THR	В	485	19.878	9.914 27.830	1.00	24.28
25	MOTA	3313		THR	В	485	19.993	7.896 29.133	1.00	23.32
	MOTA	3314	C	THR	В	485	22.017	6.881 27.188	1.00	22.13
	MOTA	3315	0	THR	В	485	22.574	6.284 28.115	1.00	23.30 23.08
	MOTA	3316	N	LEU	В	486	21.686	6.290 26.045	1.00	22.26
	ATOM	3317	7 CA	LEU	В	486	21.969	4.881 25.792	1.00 1.00	20.93
30	MOTA	3318		LEU	В	486	21.346	4.452 24.464 4.031 24.533		24.92
	ATOM	3319		LEU	В	486	19.878	4.031 24.533		21.96
	MOTA	3320		LEU	В	486	19.295	2.658 25.196		23.90
	ATOM	332		LEU	В	486	19.763	4.634 25.742		24.12
	MOTA	332		LEU	В	486	23.477 23.984	3.681 26.334		24.02
35	ATOM	332		LEU	В	486 487	24.191	5.490 25.022		24.53
	MOTA	332		ILE	В	487	25.640	5.345 24.913		25.16
	MOTA	332		ILE ILE	B B	487	26.207	6.379 23.899		25.57
	MOTA	332		ILE	В	487	27.725	6.522 24.051		24.54
40	MOTA	332		ILE	В	487	25.857	5.936 22.470		25.63
40	MOTA MOTA	332 332		ILE	В	487	26.538	4.646 22.023		25.68
			0 C	ILE	В	487	26.275	5.518 26.30	7 1.00	
	MOTA ATOM	333		ILE	В	487	27.200	4.794 26.67	1.00	
	MOTA	333		HIS	В	488	25.755	6.456 27.08		
45		333		HIS		488	26.251	6.720 28.43		
45	MOTA	333		HIS		488	25.450	7.871 29.04		
	MOTA	333		HIS		488	25.818	8.196 30.45		
	MOTA	333		HIS	В	488	25.245			
	MOTA	333		HIS	В	488	26.869			
50		333		HIS	В	488	26.927			
	MOTA	333	39 NE2	2 HIS	В	488	25.953			
	MOTA	334	40 C	HIS	В		26.123			
	ATOM	334	41 0	HIS	В		27.071			
	MOTA	334	42 N	LEU	I B		24.949			
55		334	43 CA	LEU			24.715			
	MOTA	33	44 CB	LEU			23.298			
	ATOM	33	45 CG	LEU			22.158			
	MOTA	33					20.827			
	ATOM	33					22.143			
60		33		LEU			25.718			
	MOTA	33	49 O	LEU	J B	489	26.241	1.032 30.40		

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5	ATOM	3350	N	MET	В	490	25.978	2.453 28.345	1.00	23.82
	MOTA	3351	CA	MET	В	490	26.900	1.438 27.857	1.00	26.38
	ATOM	3352	CB	MET	В	490	26.775	1.306 26.336	1.00	27.29
	ATOM	3353	CG	MET	В	490	25.418	0.776 25.895	1.00	21.68
	MOTA	3354	SD	MET	В	490	25.208	0.739 24.106	1.00	26.30
10	ATOM	3355	CE	MET	В	490	23.461	0.412 24.022	1.00	19.66
	MOTA	3356	С	MET	В	490	28.341	1.743 28.247	1.00	
	ATOM	3357	0	MET	В	490	29.109	0.833 28.574		26.42
	MOTA	3358	N	ALA	В	491	28.713	3.018 28.207	1.00	24.76
	ATOM	3359	CA	ALA	В	491	30.074		1.00	26.67
15	MOTA	3360		ALA	В	491	30.299	3.394 28.577	1.00	30.73
	ATOM	3361	C	ALA	B	491		4.882 28.335	1.00	26.66
	ATOM	3362	0	ALA	В	491	30.250	3.053 30.056	1.00	32.08
	ATOM	3363	N	LYS			31.194	2.361 30.438	1.00	34.66
	ATOM	3364	CA		В	492	29.316	3.523 30.878	1.00	33.17
20	MOTA	3365		LYS	В	492	29.354	3.267 32.309	1.00	32.82
20	MOTA		CB	LYS	В	492	28.110	3.849 32.976	1.00	36.38
		3366	CG	LYS	В	492	28.412	4.797 34.123	1.00	38.68
	ATOM	3367	CD	LYS	В	492	27.242	4.887 35.084	1.00	41.41
	ATOM	3368	CE	LYS	В	492	26.299	6.013 34.698	1.00	47.57
25	ATOM	3369	NZ	LYS	В	492	26.395	7.184 35.618	1.00	50.76
23	MOTA	3370	C	LYS	В	492	29.453	1.771 32.619	1.00	34.08
	ATOM	3371	0	LYS	В	492	30.090	1.382 33.593	1.00	34.31
	ATOM	3372	N	ALA	В	493	28.835	0.935 31.788	1.00	32.03
	MOTA	3373	CA	ALA	В	493	28.867	-0.510 31.998	1.00	30.70
30	ATOM	3374	CB	ALA	В	493	27.719	-1.181 31.245	1.00	28.80
30	MOTA	3375	C	ALA	В	493	30.201	-1.156 31.606	1.00	33.75
	MOTA	3376	0	ALA	В	493	30.402	-2.356 31.819	1.00	30.53
	ATOM	3377	И	GLY	В	494	31.102	-0.372 31.020	1.00	33.50
	ATOM	3378	CA	GLY	В	494	32.405	-0.903 30.656	1.00	33.71
35	MOTA	3379	C	GLY	В	494	32.639	-1.360 29.230	1.00	34.40
22	ATOM	3380	0	GLY	В	494	33.663	-1.989 28.950	1.00	33.13
	ATOM	3381	N	LEU	В	495	31.712	-1.056 28.326	1.00	31.76
	MOTA MOTA	3382	CA	LEU	В	495	31.859	-1.452 26.925	1.00	30.57
	ATOM	3383	CB	LEU	В	495	30.494	-1.415 26.216	1.00	30.67
40	ATOM	3384	CG	LEU	В	495	29.610	-2.675 26.256	1.00	29.59
70	ATOM	3385	CD1	LEU	В	495	29.315	-3.058 27.700	1.00	26.60
	ATOM	3386	CD2	LEU	В	495	28.307	-2.416 25.501	1.00	27.52
	ATOM	3387	C	LEU	В	495	32.829	-0.515 26.202	1.00	30.53
	ATOM	3388	0	LEU	В	495	32.855	0.688 26.468	1.00	28.14
45	ATOM	3389	N	THR	В	496	33.628	-1.064 25.291	1.00	28.03
73	ATOM	3390	CA	THR	В	496	34.567	-0.243 24.529	1.00	29.06
	ATOM	3391	CB	THR	В	496	35.511	-1.095 23.665	1.00	29.40
	ATOM	3392	OG1	THR	B	496	34.753	-1.758 22.641	1.00	30.29
		3393	CG2	THR	В	496	36.228	-2.122 24.515	1.00	28.12
50	ATOM	3394	C	THR	В	496	33.770	0.652 23.590	1.00	30.12
30	ATOM	3395	0	THR	В	496	32.580	0.433 23.380	1.00	29.74
	ATOM	3396	N	LEU	В	497	34.430	1.654 23.018	1.00	30.44
	ATOM	3397	CA	LEU	В	497	33.762	2.567 22.104	1.00	28.54
	ATOM	3398	CB	LEU	В	497	34.768	3.564 21.529	1.00	31.14
55	MOTA	3399	CG	LEU	В	497	35.209	4.719 22.434	1.00	33.58
55	ATOM	3400	CD1	LEU	В	497	36.120	5.659 21.652	1.00	31.42
	ATOM	3401	CD2	LEU	В	497	33.992	5.469 22.942	1.00	35.08
	MOTA	3402	C	LEU	В	497	33.095	1.800 20.967	1.00	27.35
	MOTA	3403	0	LEU	В	497	31.967	2.105 20.574	1.00	24.03
60	MOTA	3404	N	GLN	В	498	33.798	0.797 20.447	1.00	26.17
60	MOTA	3405	CA	GLN	В	498	33.289	-0.009 19.348	1.00	26.32
	ATOM	3406	CB	GLN	В	498	34.411	-0.876 18.771	1.00	27.25

5	n ecold	3407	CG	GLN	В	498	33.967	-1.796 17.645 1.00 32.67	
3	ATOM	3408	CD		В	498	34.965	-2.912 17.374 1.00 38.39	
	MOTA				В	498	35.737	-3.298 18.254 1.00 36.78	3
	ATOM	3409	OE1		В	498	34.953	-3.437 16.153 1.00 33.18	3
	MOTA	3410	NE2			498	32.112	-0.888 19.774 1.00 25.70)
	MOTA	3411	C	GLN	В		31.167	-1.076 19.009 1.00 25.35	
10	MOTA	3412	0	GLN	B	498		-1.434 20.986 1.00 24.03	
	MOTA	3413	N	GLN	В	499	32.173	-2.281 21.487 1.00 25.34	
	MOTA	3414	CA	GLN	В	499	31.093	-2.935 22.815 1.00 28.33	
	MOTA	3415	CB	GLN	В	499	31.501		
	MOTA	3416	CG	GLN	В	499	32.537		
15	MOTA	3417	CD	${ t GLN}$	В	499	32.913		
	ATOM	3418	OE1	GLN	В	499	33.306	-3.997 24.937 1.00 33.6	
	MOTA	3419	NE2	GLN	В	499	32.797	-6.004 24.074 1.00 30.6	
	MOTA	3420	C	GLN	В	499	29.842	-1.430 21.693 1.00 25.7	
	ATOM	3421	Ö	GLN	В	499	28.715	-1.910 21.554 1.00 26.2	
20	ATOM	3422		GLN	В	500	30.062	-0.160 22.020 1.00 23.0	
20		3423		GLN	В	500	28.989	0.793 22.256 1.00 23.5	
	MOTA	3423		GLN	В	500	29.564	2.107 22.782 1.00 26.1	
	ATOM			GLN	В	500	29.958	2.073 24.252 1.00 27.7	1
	MOTA	3425		GLN	В	500	30.812	3.262 24.641 1.00 29.3	2
	MOTA	3426			В	500	30.559	4.386 24.207 1.00 28.4	8
25	MOTA	3427		GLN		500	31.831	3.021 25.463 1.00 25.0	7
	MOTA	3428		GLN	В	500	28.151	1.074 21.015 1.00 24.2	
	MOTA	3429		GLN	В		26.923	0.949 21.053 1.00 24.4	
	MOTA	3430		GLN	В	500		1.465 19.915 1.00 23.0	
	MOTA	3431		HIS	В	501	28.790	1.739 18.724 1.00 26.9	
30	MOTA	3432	2 CA	HIS	В	501	28.004	2.577 17.697 1.00 32.0	
	MOTA	3433	3 CB	HIS	В	501	28.791	1.896 17.105 1.00 36.9	
	MOTA	3434	4 CG	HIS	В	501	29.988	2.000 2	
	ATOM	343	5 CD2	HIS	В	501	30.122	0.,20	
	MOTA	343	6 ND1	HIS	В	501	31.224	2.000	
35	MOTA	343	7 CE1	HIS	В	501	32.066		
	MOTA	343	8 NE2	HIS	В	501	31.422	0.020 20.000	
	MOTA	343	9 C	HIS	В	501	27.451	0.457 18.123 1.00 25.	
	MOTA	344	0 0	HIS	В	501	26.369	0.457 17.531 1.00 20.	
	MOTA	344		GLN	В	502	28.165	-0.648 18.317 1.00 24.	
40	MOTA	344	2 CA	GLN	В	502	27.698	-1.926 17.804 1.00 21.	
	MOTA	344		GLN	В	502	28.785	-2.996 17.953 1.00 24.	
	MOTA	344		GLN	В	502	29.796	-3.001 16.797 1.00 26.	
	MOTA	344		GLN	В	502	30.843	-4.109 16.902 1.00 27.	
	MOTA	344			В	502	30.716		
45		344			В	502	31.882		
73	ATOM	344		GLN	В	502	26.428		
	ATOM	344		GLN		502	25.464		
	MOTA	345		ARG			26.42	-2.159 19.874 1.00 20.	
		345		ARG			25.25	-2.523 20.678 1.00 22.	
50	ATOM			ARG			25.60		51
50		345		ARG			24.45		34
	MOTA	345					24.85		.18
	MOTA	345		ARG			23.74		. 62
	MOTA	345		ARG			23.74	, 5,510 110 110	. 88
	ATOM	345		ARG			23.32	, 1,00, 20,00	.40
55		34							.71
	ATOM	34					22.30	, 5,122, 20,20	.05
	MOTA	34		ARG			24.10		.87
	ATOM	34	60 O	ARG			22.94	21,500	.19
	MOTA	34	61 N	LEU			24.41	1 0,2,0 20,000	. 33
60		34	62 CA				23.37		. 25
	MOTA	34	63 CB	LEU	J E	3 504	23.97	2 2.117 19.855 1.00 16	

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5	MOTA	3464	CG	LEU	В	504	22.983	3.173 19.344	1.00	20.35
	ATOM	3465	CD1	LEU	В	504	21.930	3.449 20.427	1.00	17.97
	MOTA	3466	CD2	LEU	В	504	23.729	4.448 18.955	1.00	
	ATOM	3467	C	LEU	В	504	22.659	0.357 18.667		20.86
	ATOM	3468	0	LEU	В	504	21.433		1.00	21.22
10	ATOM	3469	N					0.478 18.566	1.00	19.28
10				ALA	В	505	23.428	-0.085 17.676	1.00	18.55
	ATOM	3470	CA	ALA	В	505	22.859	-0.473 16.396	1.00	18.20
	MOTA	3471	CB	ALA	В	505	23.973	-0.745 15.382	1.00	18.45
	ATOM	3472	С	ALA	В	505	21.986	-1.716 16.562	1.00	19.54
	ATOM	3473	0	ALA	В	505	20.871	-1.774 16.041	1.00	17.63
15	ATOM	3474	N	GLN	В	506	22.497	-2.706 17.293	1.00	20.30
	ATOM	3475	CA	GLN	В	506	21.772	-3.955 17.513	1.00	19.48
	MOTA	3476	CB	GLN	В	506	22.590	-4.893 18.409	1.00	21.75
	ATOM	3477	CG	GLN	В	506	23.798	-5.551 17.727	1.00	20.85
	MOTA	3478	CD	GLN	В	506	24.819	-6.070 18.736	1.00	26.18
20	ATOM	3479	OE1	GLN	В	506	24.564	-6.084 19.943	1.00	
	ATOM	3480	NE2	GLN	В	506	25.977	-6.499 18.245		21.83
	ATOM	3481	C	GLN	В	506	20.421		1.00	25.39
	ATOM	3482	Ö	GLN	В	506		-3.672 18.166	1.00	21.39
	ATOM	3483	N	LEU			19.396	-4.233 17.766	1.00	20.87
25	ATOM	3484	CA		В	507	20.433	-2.800 19.171	1.00	19.52
23	MOTA			LEU	В	507	19.219	-2.418 19.884	1.00	23.04
		3485	CB	LEU	В	507	19.548	-1.455 21.030	1.00	22.82
	ATOM	3486	CG	LEU	В	507	20.182	-2.011 22.313	1.00	26.12
	ATOM	3487	CD1	LEU	В	507	20.203	-0.916 23.360	1.00	29.33
20	ATOM	3488	CD2	LEU	В	507	19.415	-3.213 22.816	1.00	27.80
30	ATOM	3489	C	LEU	В	507	18.212	-1.730 18.971	1.00	22.19
	ATOM	3490	₽	LEU	В	507	17.036	-2.070 18.964	1.00	23.00
	MOTA	3491	N	LEU	В	508	18.678	-0.745 18.214	1.00	21.53
	MOTA	3492	CA	LEU	В	508	17.797	0.006 17.332	1.00	20.60
	ATOM	3493	CB	LEU	В	508	18.535	1.236 16.805	1.00	17.57
35	MOTA	3494	CG	LEU	В	508	18.934	2.218 17.913	1.00	17.67
	ATOM	3495	CD1	LEU	В	508 ·	19.566	3.446 17.301	1.00	20.04
	MOTA	3496	CD2	LEU	В	508	17.724	2.611 18.725	1.00	18.49
	ATOM	3497	С	LEU	В	508	17.235	-0.831 16.183	1.00	21.17
	ATOM	3498	0	LEU	В	508	16.118	-0.597 15.728	1.00	21.88
40	ATOM	3499	N	LEU	В	509	18.000	-1.813 15.713	1.00	21.89
	ATOM	3500	CA	LEU	В	509	17.511	-2.657 14.631		
	ATOM	3501	CB	LEU	В	509	18.603		1.00	22.81
	ATOM	3502	CG	LEU	В	509	19.645	-3.597 14.145		22.65
	ATOM	3503	CD1	LEU	В	509		-2.891 13.278	1.00	29.11
45	ATOM	3504	CD2	LEU			20.697	-3.888 12.829	1.00	25.69
	ATOM	3505	C C		В	509	18.965	-2.248 12.082	1.00	27.92
	MOTA			LEU	В	509	16.302	-3.462 15.095	1.00	23.32
		3506	0	LEU	В	509	15.409	-3.759 14.303	1.00	23.36
	ATOM	3507	N	ILE	В	510	16.264	-3.796 16.380	1.00	23.36
60	MOTA	3508	CA	ILE	В	510	15.148	-4.562 16.912	1.00	20.99
50	MOTA	3509	CB	ILE	В	510	15.448	-5.041 18.361	1.00	28.60
	MOTA	3510	CG2	ILE	В	510	14.162	-5.435 19.075	1.00	28.10
	MOTA	3511	CG1	ILE	В	510	16.383	-6.260 18.308	1.00	26.57
	MOTA	3512	CD1	ILE	В	510	17.429	-6.301 19.419	1.00	30.14
	MOTA	3513	С	ILE	В	510	13.852	-3.746 16.846	1.00	17.65
55	ATOM	3514	0	ILE	В	510	12.767	-4.308 16.759	1.00	16.11
	MOTA	3515	N	LEU	В	511	13.961	-2.421 16.867	1.00	18.12
	ATOM	3516	CA	LEU	В	511	12.772	-1.574 16.774		
	ATOM	3517	CB	LEU	В	511	13.147	-0.100 16.981	1.00	16.95
	ATOM	3518	CG	LEU	В	511	13.147		1.00	22.66
60	ATOM	3519	CD1	LEU	В	511		0.262 18.406	1.00	22.13
	ATOM	3520	CD2		В		13.404	1.751 18.652	1.00	25.29
	1+1 OF	J J Z U	CD2	LEU	Þ	511	12.830	-0.549 19.425	1.00	25.08

	WO 99/00	00014				·
				_	E 7 7	12.112 -1.771 15.397 1.00 16.65
5	ATOM	3521 C	LEU		511	10.915 -1.578 15.242 1.00 17.09
	MOTA	3522 O	LEU		511	12.901 -2.161 14.401 1.00 15.83
	ATOM	3523 N	SER	В	512	12.355 -2.408 13.072 1.00 18.66
	MOTA	3524 CA	SER	В	512	12.555
	ATOM	3525 CB	SER	В	512	13.404 -2.044 12.01
10	MOTA	3526 OG	SER	В	512	13.079
	ATOM	3527 C	SER	B	512	11.454 -3.030 13.11
	MOTA	3528 O	SER	В	512	10.373
	MOTA	3529 N	HIS	В	513	11.033
	ATOM	3530 CA	HIS	В	513	11.141 -5.000 11.00 10.00
15	MOTA	3531 CB	HIS	B	513	12.013
13	MOTA	3532 CG	HIS	В	513	13.063
	MOTA	3533 CD2	HIS	В	513	12.980 -8.364 12.868 1.00 28.40
	MOTA	3534 ND1	HIS	В	513	14.378 -7.066 13.932 1.00 28.92
		3535 CE1	HIS	В	513	15.061 -7.678 12.981 1.00 30.75
20	ATOM	3536 NE2	HIS	В	513	14.235 -8.472 12.321 1.00 30.08
20	MOTA	3537 C	HIS	В	513	9.895 -5.602 14.958 1.00 15.35
	MOTA		HIS	В	513	8.846 -6.192 14.704 1.00 14.83
	MOTA	_	ILE	В	514	10.012 -4.744 15.942 1.00 13.35
	MOTA	3539 N	ILE	В	514	8.865 -4.417 16.776 1.00 15.48
	MOTA	3540 CA	ILE	В	514 .	9.295 -3.534 17.967 1.00 20.02
25	MOTA	3541 CB		В	514	8.067 -2.918 18.650 1.00 12.84
	MOTA	3542 CG2		В	514	10.093 -4.397 18.962 1.00 22.87
	MOTA	3543 CG1		В	514	10 691 -3.641 20.115 1.00 29.62
	MOTA	3544 CD	ILE	В	514	7.797 -3.717 15.923 1.00 15.16
	MOTA	3545 C	ILE	В	514	6.606 -3.972 16.078 1.00 16.61
30	MOTA	3546 O	ARG	В	515	8.224 -2.823 15.030 1.00 16.33
	ATOM	3547 N	ARG	В	515	7.280 -2.138 14.150 1.00 17.54
	MOTA	3548 CA	ARG	В	515	8.010 -1.173 13.214 1.00 20.15
	MOTA	3549 CB	ARG		515	7.080 -0.454 12.234 1.00 21.47
	MOTA	3550 CG			515	6.407 0.749 12.891 1.00 26.05
35	MOTA	3551 CD			515	7 220 1.948 12.716 1.00 24.91
	MOTA	3552 NE			515	6 734 3.175 12.547 1.00 24.61
	MOTA	3553 CZ			515	5 424 3.393 12.522 1.00 22.46
	MOTA	3554 NH			515	7.569 4.182 12.374 1.00 23.15
	MOTA	3555 NH	ARG		515	6.545 -3.182 13.304 1.00 16.60
40		3556 C	ARG		515	5.332 -3.093 13.087 1.00 14.51
	MOTA	3557 O			516	7 298 -4.171 12.827 1.00 18.50
	MOTA	3558 N	HIS		516	6 743 -5.237 11.997 1.00 17.26
	MOTA	3559 C				7 861 -6.176 11.533 1.00 18.14
	MOTA	3560 CI				7 405 -7.223 10.568 1.00 24.87
45		3561 C				7.060 -8.521 10.754 1.00 26.64
	MOTA		D2 HIS		_	7.258 -6.978 9.220 1.00 21.82
	MOTA		O1 HIS		_	6.839 -8.078 8.619 1.00 28.42
	MOTA		E1 HI			6.711 -9.028 9.526 1.00 24.47
	MOTA		E2 HI			5.685 -6.028 12.759 1.00 16.87
50	MOTA 0	3566 C			_	4.596 -6.303 12.240 1.00 14.81
	MOTA	3567 O				5.999 -6.396 13.997 1.00 16.48
	MOTA	3568 N				3.999
	MOTA	3569 C				5.045 7.202 2.102
	ATOM	3570 C				5.701
5	5 ATOM	3571 C	G ME			0.750
_	MOTA	3572 S	D ME			7.360
	ATOM		E ME	_	3 517	0.104 ,.07 1 00 16 23
	MOTA	_			B 517	3.705
	MOTA) ME	eT l	B 517	2.000
6	O ATOM		J SE	ER :	B 518	3.934 -3.000 - 7.00 1.00 1.6 34
·	ATOM		CA SE	ER :	B 518	2.827 -4.186 15.505 1.00 16.34

5	ATOM	3578	CB	SER	В	518	3.316	-2.765-15.835	1.00	17.48
	MOTA	3579	OG	SER	В	518	2.234	-1.840 15.843	1.00	17.46
	ATOM	3580	С	SER	В	518	1.906	-4.147 14.284	1.00	14.73
	ATOM	3581	0	SER	В	518	0.688	-4.247 14.417	1.00	19.16
	ATOM	3582	N	ASN	В	519	2.474	-4.006 13.091	1.00	14.52
10	MOTA	3583	CA	ASN	В	519	1.622	-3.953 11.907	1.00	15.35
	ATOM	3584	CB	ASN	В	519	2.432	-3.509 10.698	1.00	19.21
	ATOM	3585	CG	ASN	В	519	2.700	-2.029 10.729	1.00	20.58
	ATOM	3586	OD1	ASN	В	519	1.839	-1.258 11.150		
	ATOM	3587	ND2	ASN	В	519	3.891	-1.618 10.307	1.00	26.36
15									1.00	19.62
13	MOTA	3588	С	ASN	В	519	0.911	-5.280 11.658	1.00	16.74
	ATOM	3589	0	ASN	В	519	-0.265	-5.299 11.297	1.00	20.58
	ATOM	3590	И	LYS	В	520	1.608	-6.387 11.885	1.00	18.60
	MOTA	3591	CA	LYS	В	520	0.992	-7.699 11.717	1.00	20.04
20	MOTA	3592	CB	LYS	В	520	2.038	-8.801 11.872	1.00	25.44
20	MOTA	3593	CG	LYS	В	520	3.037	-8.849 10.728	1.00	31.68
	ATOM	3594	CD	LYS	В	520	2.507	-9.663 9.558	1.00	42.56
	ATOM	3595	CE	LYS	В	520	2.186	-8.778 8.364	1.00	45.61
	ATOM	3596	NZ	LYS	В	520	1.435	-9.526 7.312	1.00	46.00
25	ATOM	3597	C	LYS	В	520	-0.099	-7.868 12.769	1.00	18.88
25	ATOM	3598	0	LYS	В	520	-1.183	-8.358 12.478	1.00	21.75
	ATOM	3599	N	GLY	В	521	0.191	-7.455 13.998	1.00	17.83
	ATOM	3600	CA	GLY	В	521	-0.792	-7.569 15.058	1.00	16.19
	ATOM	3601	C	GLY	В	521	-2.000	-6.674 14.833	1.00	16.59
20	ATOM	3602	0	GLY	В	521	-3.128	-7.060 15.125	1.00	16.57
30	MOTA	3603	N	MET	В	522	-1.766	-5.467 14.326	1.00	17.48
	MOTA	3604	CA	MET	В	522	-2.852	-4.527 14.042	1.00	18.25
	ATOM	3605	CB	MET	В	522	-2.276	-3.212 13.516	1.00	21.27
	ATOM	3606	CG	MET	В	522	-3.190	-2.018 13.707	1.00	26.97
35	MOTA	3607	SD	MET	В	522	-3.199	-1.477 15.417	1.00	30.35
33	MOTA	3608	CE	MET	В	522	-1.659	-0.605 15.475	1.00	29.86
	MOTA	3609		MET	В	522	-3.794	-5.119 12.989	1.00	18.68
	MOTA	3610		MET	В	522	-5.022	-5.008 13.097	1.00	18.80
	MOTA	3611		GLU	В	523	-3.205	-5.731 11.966	1.00	18.22
40	MOTA	3612		GLU	В	523	-3.968	-6.357 10.889	1.00	23.41
40	ATOM	3613		GLU	В	523	-3.031	-6.946 9.830	1.00	28.74
	MOTA	3614		GLU	В	523	-2.224	-5.935 9.030	1.00	34.42
	ATOM	3615		GLU	В	523	-1.095	-6.597 8.239	1.00	45.58
	MOTA	3616		GLU	В	523	-0.131	-5.894 7.857	1.00	49.48
45	MOTA	3617		GLU	В	523	-1.169	-7.825 7.999	1.00	45.97
45	ATOM	3618		GLU	В	523	-4.812	-7.482 11.465	1.00	23.98
	MOTA	3619		GLU	В	523	-5.993	-7.616 11.147	1.00	22.08
	MOTA	3620		HIS	В	524	-4.187	-8.287 12.326	1.00	23.46
	MOTA	3621		HIS	В	524	-4.846	-9.428 12.952	1.00	26.20
50	ATOM	3622		HIS	В	524		-10.245 13.743	1.00	27.26
50	ATOM	3623		HIS	В	524			1.00	30.91
	ATOM	3624		HIS	В	524	-4.308		1.00	30.90
	ATOM	3625		HIS	В	524	-5.107		1.00	28.87
	MOTA	3626		HIS	В	524	-5.461	-12.780 15.757	1.00	30.45
<i>E</i>	MOTA	3627		HIS	В	524	-4.989	-13.561 14.803	1.00	29.19
55	ATOM	3628		HIS	В	524	-5.996	-9.025 13.870	1.00	27.69
	ATOM	3629		HIS	В	524	-7.061	-9.656 13.860	1.00	25.00
	ATOM	3630		LEU	В	525	~5.777	-7.977 14.655	1.00	23.84
	MOTA	3631		LEU	В	525	-6.786	-7.492 15.588	1.00	25.77
~ ^	ATOM	3632		LEU	В	525	-6.217	-6.358 16.444	1.00	22.22
60	ATOM	3633		LEU	В	525	-7.164	-5.778 17.498	1.00	26.81
	ATOM	3634	CD1	LEU	В	525	-7.763	-6.922 18.321	1.00	23.32

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5	ATOM	3635	CD2	LEU	В	525	-6.414	-4.793	18.399	1.00	18.95
	ATOM	3636	С	LEU	В	525	-8.013	-6.995	14.842	1.00	26.84
	ATOM	3637	0	LEU	В	525	-9.154	-7.247		1.00	26.73
	ATOM	3638	N	TYR	В	526	-7.764	-6.271		1.00	26.86
	ATOM	3639	CA	TYR	В	526	-8.819	-5.726		1.00	30.89
10	MOTA	3640	CB	TYR	В	526					
10	ATOM	3641	CG				-8.201	-4.818		1.00	34.31
				TYR	В	526	-9.183	-4.223		1.00	43.50
	MOTA	3642	CD1	TYR	В	526	-10.058	-3.211		1.00	47.66
	ATOM	3643	CE1	TYR	В	526	-10.943	-2.636	10.357	1.00	48.85
	MOTA	3644	CD2	TYR	В	526	-9.218	-4.651	9.552	1.00	48.52
15	MOTA	3645	CE2	TYR	В	526	-10.098	-4.083	8.634	1.00	52.43
	MOTA	3646	CZ	TYR	В	526	-10.955	-3.077	9.043	1.00	51.67
	ATOM	3647	OH	TYR	В	526	-11.810	-2.504	8.129	1.00	57.01
	MOTA	3648	C	TYR	В	526	-9.577	-6.880		1.00	30.90
	MOTA	3649	0	TYR	В	526	-10.793	-6.829		1.00	31.48
20	MOTA	3650	N	SER	В	527	-8.849	-7.926		1.00	31.39
	ATOM	3651	CA	SER	В	527	-9.460	-9.095			
	ATOM	3652	CB .	SER	В	527				1.00	33.73
	MOTA	3653	OG	SER	В	527	-8.377	-10.048		1.00	34.13
	ATOM		C				-8.945	-11.222		1.00	43.67
25		3654		SER	В	527	-10.339	-9.813		1.00	34.34
23	MOTA	3655	0	SER	В	527	-11.446	-10.261		1.00	33.42
	ATOM	3656	N	MET	В	528	-9.840	-9.916		1.00	31.66
	MOTA	3657	CA	MET	В	528	-10.574	-10.572		1.00	29.77
	ATOM	3658	CB	MET	В	528	-9.682	-10.743	15.820	1.00	32.96
	ATOM	3659	CG	MET	В	528	-8.651	-11.859	15.699	1.00	33.47
30	MOTA	3660	SD	MET	В	528	-9.359	-13.427	15.134	1.00	38.28
	ATOM	3661	CE	MET	В	528	-10.265	-13.915	16.579	1.00	36.01
	MOTA	3662	C	MET	В	528	-11.800	-9.747		1.00	29.42
	ATOM	3663	0	MET	В	528	-12.835	-10.293		1.00	28.65
	MOTA	3664	N	LYS	В	529	-11.673	-8.429		1.00	30.64
35	ATOM	3665	CA	LYS	В	529	-12.781	-7.533		1.00	31.80
	MOTA	3666	CB	LYS	В	529	-12.323	-6.079		1.00	32.86
	ATOM	3667	CG	LYS	В	529	-13.436	-5.043			
	ATOM	3668	CD	LYS	В	529	-13.114	-3.852		1.00	36.42
	ATOM	3669	CE	LYS	В	529				1.00	41.74
40	ATOM	3670	NZ	LYS	В	529	-13.734	-2.564		1.00	43.45
.0	ATOM	3671	C				-15.221	-2.569		1.00	46.51
				LYS	В	529	-13.857	-7.840		1.00	36.60
	MOTA	3672	0	LYS	В	529	-15.049	-7.877		1.00	34.04
	ATOM	3673	N	CYS	В	530	-13.407	-8.083		1.00	40.04
15	MOTA	3674	CA	CYS	В	530	-14.286	-8.409		1.00	44.58
45	MOTA	3675	CB	CYS	В	530	-13.460	-8.535		1.00	50.64
	MOTA	3676	SG	CYS	В	530	-13.369	-7.034	9.504	1.00	67.65
	ATOM	3677	С	CYS	В	530	-15.065	-9.692	12.016	1.00	42.88
	ATOM	3678	0	CYS	В	530	-16.274	-9.741	11.807	1.00	40.15
	MOTA	3679	N	LYS	В	531	-14.360	-10.733	12.447	1.00	41.92
50	ATOM	3680	CA	LYS	В	531	-14.980	-12.023		1.00	42.60
	ATOM	3681	CB	LYS	В	531	-13.907			1.00	44.77
	ATOM	3682	С	LYS	В	531	-15.844			1.00	44.43
	MOTA	3683	0	LYS	В	531	-16.623			1.00	44.09
	ATOM	3684	N	ASN	В	532	-15.678				
55	MOTA	3685	CA	ASN	В	532				1.00	44.98
J J	MOTA	3686	CB				-16.437			1.00	44.10
				ASN	В	532	-17.833			1.00	45.14
	ATOM	3687	CG	ASN	В	532	-18.526	-9.271		1.00	46.54
	ATOM	3688	OD1	ASN	В	532	-19.729	-9.424		1.00	50.62
60	ATOM	3689	ND2	ASN	В	532	-17.771	-8.471		1.00	46.07
60	MOTA	3690	С	ASN	В	532	-16.557	-11.657		1.00	43.34
	MOTA	3691	0	ASN	В	532	-17.655	-11.994	17.321	1.00	41.42

5	ATOM	3692	N	VAL	В	533	-15.434	-12.264 17.243	1.00	43.45
	ATOM	3693	CA	VAL	В	533	-15.471		1.00	44.06
	MOTA	3694	CB	VAL	В	533	-14.170		1.00	45.56
	ATOM	3695	CG1	VAL	В	533		-14.263 16.683	1.00	45.67
	ATOM	3696	CG2	VAL	В	533		-13.644 19.045	1.00	44.16
10	MOTA	3697	C	VAL	В	533	-15.670	-12.835 19.611	1.00	43.24
10	ATOM	3698	0	VAL	В	533				
									1.00	44.21
	ATOM	3699	N	VAL	В	534		-11.511 19.755.	1.00	40.44
	MOTA	3700	CA	VAL	В	534		-10.849 21.049	1.00	37.80
1.5	MOTA	3701	CB	LAV	В	534		-11.259 22.038	1.00	36.38
15	MOTA	3702	CG1	VAL	В	534	-13.324	-10.575 21.658	1.00	34.35
	MOTA	3703	CG2	VAL	В	534	-15.021	-10.910 23.463	1.00	39.34
	MOTA	3704	C	VAL	В	534	-15.752	-9.329 20.857	1.00	37.97
	MOTA	3705	0	VAL	В	534	-15.026	-8.808 20.008	1.00	39.45
	MOTA	3706	N	PRO	В	535	-16.575	-8.597 21.625	1.00	37.81
20	MOTA	3707	CD	PRO	В	535	-17.529	-9.078 22.640	1.00	38.74
	ATOM	3708	CA	PRO	В	535	-16.608	-7.135 21.492	1.00	36.79
	MOTA	3709	CB	PRO	В	535	-17.846	-6.729 22.288	1.00	36.98
	ATOM	3710	CG	PRO	В	535	-18.004	-7.809 23.298	1.00	39.77
	MOTA	3711	С	PRO	В	535	-15:338	-6.494 22.049	1.00	33.95
25	MOTA	3712	0	PRO	В	535	-14.786	-6.963 23.040	1.00	34.93
	MOTA	3713	N	LEU	В	536	-14.881	-5.426 21.409	1.00	33.42
	MOTA	3714	CA	LEU	В	536	-13.675	-4.732 21.851	1.00	33.40
	MOTA	3715	CB	LEU	В	536	-12.829	-4.314 20.647	1.00	29.31
	MOTA	3716	CG	LEU	В	536	-12.219	-5.433 19.798	1.00	30.06
30	MOTA	3717	CD1	LEU	В	536	-11.344	-4.822 18.714	1.00	30.85
	ATOM '	3718	CD2	LEU	В	536	-11.398	-6.370 20.676	1.00	28.96
	ATOM	3719	C	LEU	В	536	-14.036	-3.498 22.666	1.00	30.50
	MOTA	3720	0	LEU	В	536	-15.024	-2.829 22.383	1.00	29.91
	ATOM	3721	N	TYR	В	537	-13.231	-3.194 23.676	1.00	28.69
35	MOTA	3722	CA	TYR	В	537	-13.494	-2.032 24.505	1.00	29.89
	MOTA	3723	CB	TYR	В	537	-12.618	-2.071 25.750	1.00	32.50
	MOTA	3724	CG	TYR	В	537	-12.849	-3.327 26.543	1.00	39.46
	MOTA	3725	CD1	TYR	В	537	-13.923	-3.431 27.421	1.00	41.90
	MOTA	3726	CE1	TYR	В	537	-14.174	-4.609 28.118	1.00	45.72
40	MOTA	3727	CD2	TYR	В	537	-12.022	-4.435 26.379	1.00	47.39
	MOTA	3728	CE2	TYR	В	537	-12.262	-5.620 27.072	1.00	49.93
	MOTA	3729	CZ	TYR	В	537	-13.340	-5.699 27.940		48.80
	MOTA	3730		TYR	В	537	-13.582	-6.872 28.624	•	53.90
	MOTA	3731	C	TYR	В	537	-13.262			27.09
45	MOTA	3732	Ō	TYR	В	537	-12.518	-0.757 22.729	1.00	26.15
	ATOM	3733	N	ASP	В	538	-13.909	0.315 24.141	1.00	26.12
	ATOM	3734	CA	ASP	В	538	-13.830		1.00	25.27
	ATOM	3735	CB	ASP	В	538	-14.748		1.00	28.85
	MOTA	3736	CG	ASP	В	538	-16.227			
50	ATOM	3737	OD1	ASP	В	538	-17.052	2.613 24.819	1.00	33.90 32.68
20	ATOM	3738	OD2	ASP	В	538				
	MOTA		C				-16.562	1.707 22.882	1.00	38.26
		3739		ASP	В	538	-12.447	2.217 23.261	1.00	25.18
	ATOM	3740	0	ASP	В	538	-12.120	2.626 22.147	1.00	26.41
55	MOTA	3741	N	LEU	В	539	-11.637	2.309 24.313	1.00	20.76
55	MOTA	3742	CA	LEU	В	539	-10.312	2.911 24.150	1.00	19.65
	MOTA	3743	CB	LEU	В	539	-9.567		1.00	17.48
	MOTA	3744	CG	LEU	В	539	-8.116	3.511 25.469	1.00	16.46
	MOTA	3745	CD1	LEU	В	539	-8.051		1.00	16.43
	MOTA	3746	CD2	LEU	В	539	-7.564		1.00	15.57
60	ATOM	3747		LEU	В	539	-9.484		1.00	16.75
	ATOM	3748	0	LEU	В	539	-8.862	2.716 22.249	1.00	20.36

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				e 1737 T	D	540	-9.487	0.803 23.239 1	.00 18	3.23
5	MOTA	_	• •		B B	540				3.05
	MOTA				ь В	540		-1.528 22.701 1	00 10	5.38
	MOTA				В	540	-8.188			9.81
	MOTA				В	540	-6.679			9.27
	ATOM				В	540	-8.473	-3.952 22.327		8.00
10	MOTA	_		LEU	В	540	-9.241	0.169 20.891	1.00 2	1.50
	ATOM		_	LEU	В	540	-8.449	0.293 19.964	1.00 2	0.41
	MOTA	_	0	LEU	В	541	-10.559		1.00 2	2.40
	MOTA	•	N	LEU	В	541	-11.164	0.419 19.413	1.00 2	3.27
	MOTA	3758	CA	LEU	В	541	-12.686			5.12
15	ATOM	3759	CB	LEU	В	541	-13.410		1.00 3	6.53
	MOTA	3760	CG	LEU	В	541	-14.910	-0.671 19.273	1.00 3	0.98
	MOTA	3761	CD1	LEU	В	541	-13.136			1.93
	MOTA	3762	CD2	LEU LEU	В	541	-10.697	1.751 18.842		22.46
	MOTA	3763	С		В	541	-10.359	1.845 17.666	1.00 2	26.29
20	MOTA	3764	0	LEU GLU	В	542	-10.694	2.781 19.680		23.96
	MOTA	3765	N	GLU	В	542	-10.248	4.106 19.270	1.00	26.91
	MOTA	3766	CA	GLU	В	542	-10.250	5.050 20.468		30.84
	MOTA	3767	CB	GLU	В	542	-11.166	6.245 20.347		37.20
	MOTA	3768	CG CD	GLU	В	542	-11.138	7.105 21.597		39.98
25	MOTA	3769	OE1	GLU	В	542	-12.223	7.385 22.144		39.92
	MOTA	3770	OE1	GLU	В	542	-10.028	7.494 22.034		38.96
	MOTA	3771 3772	C	GLU	В	542	-8.826	4.010 18.724		27.90
	MOTA	3773	0	GLU	В	542	-8.530	4.492 17.634		29.32
20	MOTA	3774		MET	В	543	7.945	3.388 19.499		26.41
30	MOTA	3775		MET	В	543	-6.552	3.237 19.107		23.53
	MOTA	3776		MET	В	543	-5.749	2.591 20.247	1.00	24.60
	ATOM ATOM	3777		MET	В	543	-5.812	3.338 21.579	1.00	26.46
	ATOM	3778		MET	В	543	-5.373	5.084 21.467	1.00	29.45
35	ATOM	3779		MET	В	543	-3.585	4.971 21.349	1.00	25.43
55	ATOM	3780		MET	В	543	-6.403	2.407 17.832	1.00	25.80
	ATOM	3781		MET	В	543	-5.535	2.686 17.004	1.00	23.59
	MOTA	3782		LEU	В	544	-7.254	1.394 17.673	1.00	27.74 26.32
	MOTA	3783		LEU	В	544	-7.202		1.00	26.32 26.75
40		3784		LEU	В	544	-8.069		1.00	28.12
-10	ATOM	3789		LEU	В	544	-8.274		1.00	26.36
	MOTA	378		LEU	В	544	-6.956		1.00	27.00
	ATOM	378	7 CD2	LEU	В		-9.330	050	1.00 1.00	26.97
	MOTA	378	8 C	LEU	В		-7.672		1.00	24.25
45		378	9 0	LEU			-7.036		1.00	30.37
	MOTA	379	0 N	ASP			-8.787		1.00	32.34
	MOTA	379	1 CA	ASF			-9.338		1.00	36.61
	MOTA	379	2 CB	ASF			-10.668			42.73
	MOTA	379	3 CG	ASI			-11.818			47.39
5(MOTA (379	4 OD1				-12.858			46.96
	MOTA	379	5 OD2				-11.676			31.27
	MOTA	379	6 C	ASI			-8.382			30.53
	MOTA	379	7 0	ASI			-8.443			29.02
	MOTA	379		AL			-7.50			31.21
5	5 ATOM	379	99 CA	AL			-6.54			30.98
	MOTA	380		AL			-5.64°			32.14
	ATOM	380		AL			-5.69			33.78
	ATOM	380		AL			-5.18 -5.55			32.27
	MOTA	380		HI		547	-5.55 -4.77			37.73
6	MOTA 0	38			-	B 547	-4.77 -3.99			35.83
	MOTA	38	05 CB	HI	ا ن ا	B 547	-3.99			

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_	» EPOM	3006	CG	HIS	В	547	-2.796	1.968 13.269 1.00 34.54			
		3806 3807	CD2	HIS	В	547	-2.698	2.553 14.486 1.00 30.23			
	MOTA MOTA	3808	ND1	HIS	В	547	-1.502	1.755 12.840 1.00 34.23			
	MOTA	3809	CEL	HIS	В	547	-0.659	2.193 13.760 1.00 36.72			
	MOTA	3810	NE2	HIS	В	547	-1.360	2.681 14.768 1.00 31.48			
10	ATOM	3811	C	HIS	В	547	-5.649	2.286 10.735 1.00 43.69			
10	MOTA	3812	Ō	HIS	В	547	-5.178	2.152 9.606 1.00 46.04			
	ATOM	3813	N	ARG	В	548	-6.919	2.020 11.019 1.00 48.35 1.551 9.993 1.00 54.74			
	MOTA	3814	CA	ARG	В	548	-7.843				
	MOTA	3815	CB	ARG	В	548	-8.522				
15	MOTA	3816	С	ARG	В	548	-8.886				
	MOTA	3817	0	ARG	В	548	-8.580	3.812 9.672 1.00 62.81 2.186 9.422 1.00 64.81			
	MOTA	3818	N	LEU	В	549	-10.116 -11.204	3.109 9.112 1.00 67.59			
	MOTA	3819	CA	LEU	В	549	-12.478	2.327 8.799 1.00 68.06			
	MOTA	3820	CB	LEU	В	549 549	-11.449	4.069 10.275 1.00 69.12			
20	MOTA	3821	C	LEU	B B	549	-11.451	5.297 10.036 1.00 68.96			
	MOTA	3822		LEU	В	549	-11.634	3.579 11.412 1.00 70.70			
	MOTA	3823		DES	В	600	-4.547	-6.077 22.000 1.00 18.55			
	HETATM	3824 3825		DES	В	600	-3.163	-6.365 21.467 1.00 17.72			
25	HETATM	3825		DES	В	600	-2.897	-7.853 21.381 1.00 21.17			
25	HETATM HETATM	3827		DES	В	600	-3.719	-8.551 20.374 1.00 22.05			
	HETATM	3828		DES	В	600	-3.405	-8.481 18.998 1.00 21.32			
	HETATM	3829		DES	В	600	-4.239	-9.095 18.063 1.00 21.61 -9.771 18.509 1.00 24.89			
	HETATM	3830		DES	В	600	-5.388	5.772 20.000			
30	HETATM	3831	L OP3	DES	В	600		-10.339 17.600 1.00 24.94 -9.858 19.860 1.00 24.08			
	\mathtt{HETATM}	3832		DES	B	600	-5.718 -4.877	-9.240 20.791 1.00 24.67			
	HETATM	3833		DES	В	600 600	-1.998	-8.460 22.190 1.00 16.67			
	HETATM			DES	B B	600	-1.330	-7.834 23.325 1.00 15.39			
	HETATM			DES DES	В	600	-2.054	-7.642 24.522 1.00 17.62			
35	HETATM			DES		600	-1.433	-7.072 25.634 1.00 16.16			
	HETATM HETATM			DES		600	-0.077	-6.685 25.542 1.00 20.04			
	HETATM			DES		600	0.509	-6.113 26.655 1.00 15.55			
	HETATM			DES	В	600	0.669	-6.866 24.353 1.00 18.94 -7.440 23.241 1.00 15.20			
40	HETATM			DES			0.035	7.110 2012			
	HETATM		2 C8	DES			-1.642	J. J 0 J 2			
	HETATM	1 384	.3 C9	DES			-0.440	-10.009 20.998 1.00 11.63 -22.994 25.273 1.00 55.80			
	HETATN	1 384		CBM			4 799	-24.187 25.003 1.00 55.56			
	HETAT			CBN			-4.789 -4.798	-22.559 26.552 1.00 56.04			
45				CBN CBN			-5.468	-21.960 24.264 1.00 57.04			
	HETAT			CBI			-15.278	-5.124 10.243 1.00 87.39			
	HETATI			CBI			-15.852	-5.086 9.064 1.00 87.68			
	HETATI HETATI						-15.832	-4.291 11.201 1.00 86.22			
50			-				-14.207	-5.886 10.628 1.00 87.65			
30	ATOM	38				687		-20.030 -2.211 1.00 63.34			
	MOTA	38		HI		687	10.133				
	MOTA	38		HI	s (C 687	11.204	mag 7 00 CE 42			
	ATOM	38		HI		C 687	7.944	17.505 51.44			
5.5		38	56 CA			C 687	9.424	177,101 0,000			
	MOTA	38	57 N	LY		C 688	9.533	7 20.202 510.0			
	MOTA	38	58 CF			C 688	10.101	0 -21.540 -7.901 1.00 61.76			
	MOTA		59 CE			C 688	8.980	0 -20.127 -7.827 1.00 57.47			
	MOTA		60 C	Γλ		C 688	12 25	3 -20.379 -7.858 1.00 57.64			
6			61 O	II LY		C 689	10.51	1 -19.103 -8.482 1.00 55.74			
	MOTA	38	862 N	TT	سد						
						.	198	VDI II E 26)			

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5	MOTA	3863	CA	ILE	С	689	11.326	-18.212 -9.306	1.00	53.09
	ATOM	3864	CB	ILE	С	689	10.496	-17.057 -9.889	1.00	53.83
	MOTA	3865	CG2	ILE	С	689	11.334	-16.286-10.902	1.00	54.55
	MOTA	3866	CG1	ILE	С	689	9.229	-17.603-10.551	1.00	52.90
	MOTA	3867	CD1	ILE	C	689	8.406	-16.550-11.258	1.00	50.45
10	ATOM	3868	С	ILE	С	689	12.513	-17.611 -8.560	1.00	50.82
	MOTA	3869	0	ILE	С	689	13.616	-17.550 -9.097	1.00	51.28
	MOTA	3870	N	LEU	С	690	12.288	-17.162 -7.329	1.00	48.01
	MOTA	3871	CA	LEU	С	690	13.362	-16.570 -6.534	1.00	47.33
	MOTA	3872	CB	LEU	C	690	12.812	-16.058 -5.199	1.00	42.51
15	ATOM	3873	CG	LEU	C	690	13.835	-15.501 -4.206	1.00	
	ATOM	3874	CD1	LEU	Ċ	690	14.575	-14.324 -4.831	1.00	40.67
	MOTA	3875	CD2	LEU	Ċ	690	13.128	-15.078 -2.926		39.95
	MOTA	3876	C	LEU	Ċ	690	14.445	-17.615 -6.282	1.00	38.77
	ATOM	3877	Ō	LEU	Ċ	690	15.643	-17.340 -6.393	1.00	48.87
20	ATOM	3878	N	HIS	Ċ	691	14.001	-18.818 -5.939	1.00	46.71
	ATOM	3879	CA	HIS	C	691	14.886	-19.946 -5.675	1.00	51.36
	MOTA	3880	CB	HIS	Ċ	691	14.042	-21.203 -5.460	1.00	53.35
	ATOM	3881	CG	HIS	C	691	14.655		1.00	58.64
	ATOM	3882	CD2	HIS	C	691	15.503	-22.195 -4.526	1.00	62.94
25	MOTA	3883	ND1	HIS	C	691	14.392	-23.227 -4.751	1.00	64.95
	ATOM	3884	CE1	HIS	C	691	15.053	-22.202 -3.173	1.00	65.49
	ATOM	3885	NE2	HIS	C	691	15.733	-23.195 -2.605	1.00	68.18
	ATOM	3886	C	HIS	C	691		-23.833 -3.540	1.00	68.77
	ATOM	3887	0	HIS	C	691	15.824	-20.162 -6.861	1.00	52.19
30	ATOM	3888	N	ARG	C	692	17.048	-20.153 -6.717	1.00	47.53
	ATOM	3889	CA	ARG	C	692	15.222	-20.350 -8.032	1.00	52.37
	MOTA	3890	CB	ARG	C	692	15.949	-20.586 -9.271	1.00	52.90
	ATOM	3891	CG	ARG	C	692	14.955	-20.832-10.410	1.00	54.04
	ATOM	3892	CD	ARG	C	692 692	15.575	-20.826-11.797	1.00	57.52
35	MOTA	3893	NE	ARG	C	692	14.528	-21.048-12.874	1.00	58.25
55	ATOM	3894	CZ	ARG	C	692 692	14.375	-19.878-13.732	1.00	61.43
	ATOM	3895	NH1	ARG	C	692 692	13.218	-19.260-13.951	1.00	64.32
	ATOM	3896	NH2	ARG	C	692 692	12.108	-19.706-13.378	1.00	63.22
	ATOM	3897	C	ARG	C	692	13.171 16.873	-18.197-14.746	1.00	65.93
40	ATOM	3898	0	ARG	C	692		-19.434 -9.639	1.00	53.09
, 0	ATOM	3899	Ŋ	LEU	C	693	18.047 16.338	-19.644 -9.956	1.00	53.06
	ATOM	3900	CA	LEU	C	693		-18.217 -9.607	1.00	50.73
	ATOM	3901	CB	LEU	C	693		-17.039 -9.945	1.00	49.53
	ATOM	3902	CG	LEU	C	693		-15.784 -9.881	1.00	49.56
45	ATOM	3903	CD1	LEU	C	693		-15.245-11.239	1.00	49.78
	ATOM	3904	CD2	LEU	C	693	15.219		1.00	50.30
	ATOM	3905	C	LEU	C	693	14.728		1.00	48.79
	ATOM	3906	0	LEU	C		18.318		1.00	48.38
	ATOM	3907	И	LEU	C	693	19.382		1.00	46.35
50	ATOM	3908	CA	LEU	C	694	18.135	· · · · · · · · · · · · · · · · · · ·	1.00	46.74
50	ATOM	3909	CB	LEU		694	19.204		1.00	49.41
	ATOM	3910	CG		C	694	18.634		1.00	45.20
	ATOM			LEU	C	694	18.222		1.00	40.19
	ATOM	3911 3912	CD1 CD2	LEU	C	694	17.456		1.00	41.65
55	ATOM			LEU	C	694	19.453		1.00	35.91
رر		3913	C	LEU	C	694		-18.417 -7.058	1.00	54.15
	ATOM ATOM	3914	0	LEU	C	694		-18.320 -6.776	1.00	53.55
		3915	N	GLN	C	695		-19.498 -7.619	1.00	57.44
	ATOM	3916	CA	GLN	C	695		-20.685 -7.959	1.00	62.46
60	ATOM ATOM	3917	CB	GLN	C	695		-21.853 -8.304	1.00	61.95
00		3918	CG	GLN	C	695		-23.010 -7.311	1.00	61.49
	ATOM	3919	CD	GLN	С	695	18.454	-24.053 -7.490	1.00	62.78

_			0.71	CT N	~	C05	10 262	-24.928 -6.653	1.00	63.33
5	MOTA		OE1	GLN	С	695		-23.969 -8.608	1.00	60.37
	ATOM		NE2	GLN	C	695		-20.414 -9.149	1.00	65.13
	ATOM		C	GLN	C	695		-20.414 -9.149	1.00	65.87
	MOTA	3923	0	GLN	C	695		-19.824-10.197	1.00	67.67
	MOTA		N	ASP	C	696	20.761		1.00	70.66
10	MOTA	3925	CA	ASP	C	696	21.492	-19.500-11.420		
	MOTA	3926	CB	ASP	С	696	20.801	-18.348-12.151	1.00	71.06
	ATOM	3927	CG	ASP	С	696	20.127		1.00	71.70
	MOTA	3928	OD1	ASP	C	696	20.637		1.00	72.47
	MOTA	3929	OD2	ASP	С	696	19.086		1.00	71.41
15	MOTA	3930	С	ASP	С	696		-19.132-11.169	1.00	72.41
	MOTA	3931	0	ASP	С	696	23.245	-18.115-10.541	1.00	72.56
	MOTA	3932	N	SER	C	697	23.859		1.00	74.67
	MOTA	3933	CA	SER	С	697	25.291		1.00	76.45
	MOTA	3934	CB	SER	С	697	26.019	-21.076-11.377	1.00	76.00
20	MOTA	3935	C	SER	С	697	25.841	-18.960-12.696	1.00	78.44
	MOTA	3936	0	SER	C	697	26.286	-17.809-12.489	1.00	79.20
	MOTA	3937	TXO	SER	C	697	25.818	-19.510-13.820	1.00	80.07
	MOTA	3938	CB	LYS	D	686	-14.070	13.661 16.843	1.00	50.28
	MOTA	3939	С	LYS	D	686	-13.682	14.418 19.199	1.00	51.59
25	MOTA	3940	0	LYS	D	686	-12.629	14.738 19.759	1.00	50.42
	MOTA	3941	N	LYS	D	686	-12.910		1.00	50.43
	ATOM	3942	CA	LYS	D	686	-13.976		1.00	50.62
	MOTA	3943	N	HIS	D	687	-14.617		1.00	49.91
	ATOM	3944	CA	HIS	D	687	-14.447		100	51.28
30	MOTA	3945	CB	HIS	D	687	-15.806		1.00	54.12
	MOTA	3946	CG	HIS	D	687	-15.713		1.00	60.06
	MOTA	3947	CD2	HIS	D	687	-15.418		1.00	61.05
	MOTA	3948	ND1	HIS	D	687	-15.911		1.00	62.39
	MOTA	3949	CE1	HIS	D	687	-15.741		1.00	62.76
35	ATOM	3950	NE2	\mathtt{HIS}	D	687	-15.441			63.46
	MOTA	3951	C	HIS	D	687	-13.691			49.55
	ATOM	3952	0	HIS	D	687	-14.099			50.84
	MOTA	3953	N	LYS	D	688	-12.593			44.00
	MOTA	3954	CA	LYS	D	688	-11.784			40.31
40	MOTA	3955	CB	LYS	D	688	-10.446			41.42
	MOTA	3956	CG	LYS	D	688	-10.513			42.76
	MOTA	3957		LYS	D	688	-9.123			38.€€
	MOTA	3958		LYS	D	688	-9.162			38.28
	MOTA	3959		LYS	D	688	-7.894			31.58
45	MOTA	3960		LYS	D	688	-11.506			36.70
	ATOM	3961		LYS	D	688	-11.271			
	MOTA	3962		ILE	D	689	-11.549			33.06
	MOTA	3963	CA	ILE	D	689	-11.255			
	MOTA	3964	CB	ILE	D	689	-11.438			
50	MOTA	3965	CG2	ILE	D	689	-10.725			
	MOTA	3966	CG1	ILE	D	689	-12.927			
	ATOM	3967	CD1	ILE	D	689	-13.308			
	MOTA	3968	C	ILE	D	689	-9.790			
	ATOM	3969	0	ILE	D	689	-9.405			
55	ATOM	3970	N	LEU	D	690	-8.985			
	MOTA	3971		LEU	D	690	-7.563	9.348 24.549		
	MOTA	3972		LEU	D	690	-6.903	9.021 23.200	1.00	
	MOTA	3.973		LEU	D	690	-5.433	9.387 22.992	1.00	
	ATOM	3974		LEU	D	690	-4.59		3 1.00	24.03
60	ATOM	3975		LEU	D	690	-4.95	6 8.898 21.616	1.00	20.87
	ATOM	3976		LEU	D	690	-7.34	4 10.823 24.903	2 1.00	26.64

5	ATOM	3977	0	LEU	D	690	-6.408	11.165 25.625	1.00	28.34
	ATOM	3978	N	HIS	D	691	-8.206	11.694 24.383	1.00	27.77
	MOTA	3979	CA	HIS	D	691	-8.107	13.125 24.665	1.00	29.16
	MOTA	3980	CB	HIS	D	691	-9.156	13.907 23.861	1.00	30.89
	MOTA	3981	CG	HIS	D	691	-8.903	13.935 22.386	1.00	37.09
10	ATOM	3982	CD2	HIS	D	691	-7.750	14.000 21.679	1.00	41.39
	ATOM	3983	ND1	HIS	D	691	-9.920	13.906 21.458	1.00	41.65
	MOTA	3984	CE1	HIS	D	691	-9.407	13.953 20.242	1.00	44.64
	MOTA	3985	NE2	HIS	D	691	-8.091	14.010 20.347	1.00	41.94
	MOTA	3986	С	HIS	D	691	-8.338	13.373 26.159	1.00	26.65
15	MOTA	3987	0	HIS	D	691	-7.602	14.120 26.802	1.00	24.50
	MOTA	3988	И	ARG	D	692	-9.371	12.742 26.703	1.00	25.70
	MOTA	3989	CA	ARG	D	692	-9.691	12.912 28.114	1.00	29.11
	ATOM	3990	CB	ARG	D	692	-10.959	12.134 28.472	1.00	30.84
	ATOM	3991	CG	ARG	D	692	-11.255	12.129 29.963	1.00	41.63
20	ATOM	3992	CD	ARG	D	692	-12.502	11.327 30.290	1.00	48.83
	ATOM	3993	NE	ARG	D	692	-13.618	12.198 30.647	1.00	54.50
	ATOM	3994	CZ	ARG	D	692	-14.498	12.677 29.774	1.00	59.37
	MOTA	3995	NH1	ARG	D	692	-14.392	12.371 28.486	1.00	60.97
	ATOM	3996	NH2	ARG	D	692	-15.483	13.464 30.188	1.00	59.07
25	MOTA	3997	C	ARG	D	692	-8.548	12.451 29.011	1.00	28.30
	MOTA	3998	0	ARG	D	692	-8.139	13.167 29.929	1.00	26.50
	MOTA	3999	N	LEU	D	693	-8.030	11.259 28.737	1.00	24.87
	MOTA	4000	CA	LEU	D	693	-6.943	10.705 29.536	1.00	27.17
	ATOM	4001	CB	LEU	D	693	-6.674	9.254 29.116	1.00	28.45
30	ATOM	4002	CG	LEU	D	693	-7.844	8.300 29.391	1.00	30.40
	ATOM	4003	CD1	LEU	D	693	-7.575	6.932 28.778	1.00	34.79
	ATOM	4004	CD2	LEU	D	693	-8.043	8.171 30.894	1.00	32.02
	ATOM	4005	C	LEU	D	693	-5.670	11.539 29.440	1.00	25.96
	MOTA	4006	0	LEU	D	693	-4.948	11.700 30.428	1.00	27.01
35	MOTA	4007	N	LEU	D	694	-5.395	12.080 28.257	1.00	25.33
	ATOM	4008	CA	LEU	D	694	-4.207	12.906 28.062	1.00	27.22
	ATOM	4009	CB	LEU	D	694	-3.948	13.126 26.572	1.00	24.61
	ATOM	4010	CG	LEU	D	694	-3.118	12.080 25.825	1.00	22.20
	MOTA	4011	CD1	LEU	D	694	-3.230	12.332 24.324	1.00	21.13
40	MOTA	4012	CD2	LEU	D	694	-1.666	12.148 26.275	1.00	21.34
	MOTA	4013	С	LEU	D	694	-4.336	14.270 28.742	1.00	32.40
	ATOM	4014	0	LEU	D	694	-3.339	14.889 29.102	1.00	31.55
	. ATOM	4015	N	GLN	D	695	-5.570	14.733 28.915	1.00	36.93
	MOTA	4016	CA	${ t GLN}$	D	695	-5.820	16.032 29.528	1.00	43.18
45	ATOM	4017		GLN	D	695	-7.022	16.694 28.862	1.00	40.48
	ATOM	4018	CG	${ t GLN}$	D	695	-6.772	17.071 27.422	1.00	37.99
	MOTA	4019		${ t GLN}$	D	695	-7.943	17.764 26.795	1.00	35.86
	MOTA	4020		GLN	D	695	-7.863	18.895 26.342	1.00	38.84
	MOTA	4021		GLN	D	695	-9.082	17.060 26.757	1.00	31.62
50	MOTA	4022		${ t GLN}$	D	695	-6.049	16.009 31.034	1.00	48.74
	MOTA	4023		GLN	D	695	-6.119	17.065 31.660	1.00	51.25
	MOTA	4024		ASP	D	696	-6.175	14.818 31.611	1.00	54.01
	ATOM	4025		ASP	D	696	-6.398	14.702 33.047	1.00	62.23
	ATOM	4026		ASP	D	696	-6.217	13.238 33.485	1.00	63.97
55	ATOM	4027		ASP	D ·	696	-7.527	12.467 33.475	1.00	67.72
	ATOM	4028		ASP	D	696	-8.528	12.996 32.941	1.00	68.11
	MOTA	4029		ASP	D	696	-7.552	11.333 34.003	1.00	68.95
	ATOM	4030		ASP	D	696	-5.456	15.622 33.840	1.00	65.60
	MOTA	4031		ASP	D	696	-4.312	15.189 34.134	1.00	68.33
60	MOTA	4032		ASP	D	696	-5.874	16.755 34.140	1.00	69.20
	HETATM	4033	0	нон		1	16.153	-0.605 -4.425	1.00	17.11

5	HETATM	4034	0	нон	2	16.570	-5.304-16.560	14.00	21.44
	HETATM	4035	0	нон	3	18.526	0.742 -4.495	1.00	23.43
	HETATM	4036	0	HOH	4	13.647	-2.187 8.588	1.00	25.82
	HETATM	4037	0	нон	5	9.778	-5.825 2.509	1.00	20.58
	HETATM	4038	0	HOH	6	17.072	-3.605 -8.015	1.00	18.38
10	HETATM	4039	0	нон	7	24.920	-1.689 -2.780	1.00	25.74
	HETATM	4040	0	нон	8	7.321	-5.649 5.061	1.00	24.11
	HETATM	4041	0	нон	9	25.976	-3.535 15.158	1.00	26.78
	HETATM	4042	0	нон	10	15.088	-7.006-15.192	1.00	19.64
	HETATM	4043	0	НОН	11	14.070	0.925 -5.953	1.00	20.55
15	HETATM	4044	0	нон	12	18.008	3.407 -6.654	1.00	32.30
	HETATM	4045	0	HOH	13	31.949	-8.393 13.487	1.00	30.64
	HETATM	4046	0	нон	14	19.625	-2.804 -4.279	1.00	24.45
	HETATM	4047	0	нон	15	11.741	1.079-21.140	1.00	25.87
	HETATM	4048	0	нон	16	25.067	13.951 14.153	1.00	31.07
20	HETATM	4049	0	HOH .	17	15.501	1.323-10.393	1.00	21.01
	HETATM	4050	0	нон	18	13.880	3.349-11.482	1.00	24.28
	HETATM	4051	0	нон	19	17.591	. 0.979 -8.828	1.00	35.26
	HETATM	4052	0	нон	20	23.682	-2.041 -0.314	1.00	37.90
	HETATM	4053	0	нон	21	15.754	9.496 11.841	1.00	39.44
25	HETATM	4054	0	нон	22	-4.943	7.574 -3.066	1.00	37.67
	HETATM	4055	0	нон	23	6.877	0.354-15.982	1.00	36.92
	HETATM	4056	0	нон	24	15.806	-4.002 8.671	1.00	30.38
	HETATM	4057	0	нон	25	17.185	-3.158 -5.321	1.00	28.89
	HETATM	4058	0	нон	26	17.572	9.249 17.009	1.00	30.15
30	HETATM	4059	0	нон	27	24.096	-2.929 11.604	1.00	31.37
	HETATM	4060	0	нон	28	22.324	-5.871-11.980	1.00	32.74
	HETATM	4061	0	HOH	29	27.547	-12.361 -0.801	1.00	36.61
	HETATM	4062	0	HOH	30	11.173	13.442 -2.719	1.00	35.41
	HETATM	4063	0	HOH	31	15.438	-9.527 5.483	1.00	29.88
35	HETATM	4064	0	HOH	32	9.946	-6.564 5.983	1.00	35.05
	HETATM	4065	0	HOH	33	7.599	11.680-15.261	1.00	38.68
	HETATM	4066	0	HOH	34	20.112	10.503 -5.109	1.00	42.66
	HETATM	4067	0	HOH	35	15.972	10.343 14.897	1.00	41.73
	HETATM	4068	0	HOH	36	22.401	-5.914 -9.527	1.00	28.08
40	HETATM	4069	0	HOH	37	16.128	-0.899 -8.109	1.00	33.13
	HETATM	4070		нон	38	3.581	15.655 -3.706	1.00	41.37
	HETATM	4071	0	нон	39	31.900	13.545 21.339	1.00	37.79
	HETATM	4072	0	нон	40	20.058	-7.530 14.119	1.00	47.51
	HETATM	4073	0	HOH	41	34.634	6.668 15.632	1.00	29.24
45	HETATM	4074	0	нон	42	17.968	10.511 -9.085	1.00	44.60
	HETATM	4075		HOH	43	23.258		1.00	44.10
	HETATM	4076		нон	44	4.034	-1.472 27.521	1.00	15.22
	HETATM	4077		HOH	45	-5.943	-0.018 36.088	1.00	21.11
	HETATM	4078		нон	46	6.084	-1.509 29.478	1.00	19.51
50	HETATM	4079		нон	47	9.762	1.061 15.621	1.00	27.74
	HETATM	4080		HOH	48	1.804	0.717 17.260	1.00	20.97
	HETATM	4081		HOH	49	0.929	0.421 30.281	1.00	19.64
	HETATM	4082		HOH	50	9.627	4.271 31.231	1.00	19.02
	HETATM	4083		нон	51	2.121	-0.261 13.654	1.00	26.09
55	HETATM	4084		HOH	52	20.060	10.275 17.711	1.00	25.49
	HETATM	4085		HOH	53	-6.786	0.736 33.483	1.00	22.34
	HETATM	4086		HOH	54	2.751	-4.136 27.760	1.00	19.93
	HETATM	4087		нон	55	5.994	-4.079 31.292	1.00	32.27
	HETATM	4088		HOH	56	19.416	16.921 21.645	1.00	25.54
60	HETATM	4089		HOH	57	4.833	2.325 29.006	1.00	19.00
	HETATM	4090	0	нон	58	-7.638	-8.931 37.809	1.00	24.79

5	HETATM	4091	0	нон	59	28.442	-4.673 21.875	1.00	24.32
3	HETATM	4092	0	нон	60	1.094	-4.893 32.100	1.00	24.27
	HETATM	4093	0	нон	61	0.905	-7.306 32.783	1.00	21.33
	HETATM	4094	0	нон	62	3.396	-2.971 32.306	1.00	26.13
	HETATM	4095	0	нон	63	10.363	4.576 28.391	1.00	33.43
10	HETATM	4096	0	нон	64	19.551	-6.473 16.597	1.00	35.38
10	HETATM	4097	0	нон	65	-2.888	-19.627 15.665	1.00	27.99
	HETATM	4098	0	нон	66	-7.275	-9.745 31.077	1.00	27.00
	HETATM	4098	0	нон	67	10.189	3.580 16.510	1.00	24.19
	HETATM	4100	0	нон	68	2.741	0.716 28.382	1.00	16.48
15	HETATM	4101	0	нон	69	23.522	-4.323 13.943	1.00	27.48
13	HETATM	4101	0	нон	70	17.133	8.133 19.686	1.00	32.24
		4102	_	нон	71	-0.295	4.535 35.884	1.00	33.42
	HETATM		0	HOH	71 72	9.519	10.828 34.842	1.00	29.38
	HETATM	4104	0	HOH	73	6.291	14.878 29.070	1.00	28.21
20	HETATM	4105	0	нон нон	73 74	-1.721	6.480 13.381	1.00	49.91
20	HETATM	4106 4107	-	нон нон	7 4 75		-15.427 26.194		
	HETATM		0	HOH	75 76	10.091 5.029	7.461 17.718	1.00	24.17 18.91
	HETATM	4108		HOH	77	3.758	2.086 14.306	1.00	28.28
	HETATM	4109	0	нон нон	7 7 78	-1.390	-18.739 33.183	1.00	
25	HETATM	4110	_	нон нон	78 79		-8.687 32.119		41.11 36.21
23	HETATM	4111	0	HOH	79 80	12.703 22.270		1.00	
	HETATM	4112	0	HOH	81		-6.451 14.844	1.00	33.21 23.59
	HETATM	4113	0	HOH	82	1.458 1.759	4.605 34.026 -2.158 30.374		23.59
	HETATM	4114	0					1.00	
20	HETATM	4115	0	нон	83	.6.153	-21.372 23.188	1.00	31.14
30	HETATM	4116	0	нон	84	36.525	0.463 20.792	1.00	45.26
	HETATM	4117 4118	0	НОН НОН	85 86	13.832	9.696 13.792 6.635 24.924	1.00	33.12
	HETATM		0		86 87	31.166 8.844	-10.389 34.180	1.00	35.19 48.80
	HETATM	4119	0	HOH	88	9.581	-6.956 34.136	1.00	
35	HETATM	4120	0	нон	89	-1.563	15.887 27.596	1.00	42.95
33	HETATM	4121		НОН НОН	90	-5.286	10.345 32.757	1.00	39.35 35.20
	HETATM	4122 4123		HOH	90 91	15.035	0.607 13.339	1.00	29.53
	HETATM		0		91	-10.984	-1.500 30.272		29.53
	HETATM HETATM	4124 4125	0	НОН НОН	92 93	-7.239	-0.271 -1.207	1.00	
40			_	нон нон	93 94			1.00	48.98
40	HETATM	4126 4127			9 4 95	18.022	-4.902 34.286 -6.319 19.920	1.00	35.28
	HETATM HETATM	4127		НОН НОН	95 96	29.347 -14.309	-19.369 20.945	1.00	37.20 30.23
				нон	96 97				38.79
	HETATM	4129			97 98	31.496 26.567	4.614 18.716 9.759 25.629	1.00	
45	HETATM	4130		нон нон	98 99			1.00	29.72 38.08
43	HETATM	4131				2.848	14.531 1.134 5.699 -7.953	1.00	
	HETATM	4132		нон	100	-9.373		1.00	53.23
	HETATM	4133		нон	101	-10.137	-0.553 -6.742	1.00	47.72
	HETATM	4134	0	HOH	102	10.558	-10.363 15.403	1.00	40.97

5	***************************************	4148	0	нон	116	7.170	15.583 2.599	1.00	43.69
3	HETATM		0	нон	117	-1.966	10.606 3.572	1.00	52.63
	HETATM	4149	0	нон	118	29.030	10.644 6.707	1.00	42.54
	HETATM	4150		нон	119	0.468	4.354 8.374	1.00	38.69
	HETATM	4151	0		120	29.086	17.119 19.272	1.00	45.51
4.0	HETATM	4152	0	нон	121	24.614	17.609 20.174	1.00	53.55
10	HETATM	4153	0	нон		-15.318	0.362 26.686	1.00	36.77
	HETATM	4154	0	нон	122	-3.857	-24.786 28.325	1.00	39.64
	HETATM	4155	0	нон	123	21.728	22.178 31.983	1.00	43.73
	HETATM	4156	0	нон	124		-7.370 21.642	1.00	40.53
	HETATM	4157	0	нон	125	31.650		1.00	32.31
15	HETATM	4158	0	HOH	126	25.421	10.436 21.161		37.77
	HETATM	4159	0	HOH	127	10.317	-9.457 12.998	1.00	
	HETATM	4160	0	нон	128	22.723	14.887 15.427	1.00	47.90
	HETATM	4161	0	нон	129	6.702	9.556 37.596	1.00	47.81
	HETATM	4162	0	HOH	130	27.987	13.557 7.167	1.00	41.15
20	HETATM	4163	0	HOH	131	30.798	16.499 7.588	1.00	58.47
	HETATM	4164	0	HOH	132	10.071	-0.571-20.393	1.00	38.79
	HETATM	4165	0	HOH	133	9.562	8.334-21.392	1.00	36.80
	HETATM	4166	0	HOH	134	6.712	6.058 8.822	1.00	37.43
	HETATM	4167	0	HOH	135	5.927	8.454 10.594	1.00	42.34
25	HETATM	4168	0	HOH	136	4.472	6.306 10.973	1.00	37.35
	HETATM	4169	0	HOH	137	6.792	7.721 7.051	1.00	47.23
	HETATM	4170	0	нон	138	24.513	11.582 33.724	1.00	45.55
	HETATM	4171	0	HOH	139	-2.528	-20.361 12.354	1.00	52.13
	HETATM	4172	0	HOH	140	-7.864	7.706 19.248	1.00	47.82
30	HETATM	4173	0	HOH	141	11.577	-16.962 24.398	1.00	39.43
	HETATM	4174	. 0	HOH	142	18.087	12.263 -5.507	1.00	33.36
	HETATM	4175	0	HOH	143	-6.816	-14.190 10.674	1.00	51.32
	HETATM	4176	0	HOH	144	-7.377		1.00	57.11
	HETATM	4177		нон	145	-5.379	-20.107 32.689	1.00	43.01
35	HETATM	4178	3 0	HOH	146	8.766	-7.947-16.274	1.00	49.96
23	HETATM	4179		нон	147	10.946	-7.937-18.142	1.00	55.67
	END								

5 Appendix 3

Atomic Coordinates for Human ER α Complexed With OHT

Atomic Cool dinates for Manual 2200 Company											
10	CRYST1	58.24	2 58.2	42 2	77.467	90.00	90.00 12	0.00 P	65 2	2 12	
10	ODTC V1	1 00	0000	0.000	000	0.00000	0.0000	0			
	ORIGX1		0000	1.0000		0.000000		0			
	ORIGX2		0000	0.000		1.000000					
	ORIGX3			0.009		0.000000					
	SCALE1		17170	0.019		0.000000					
15	SCALE2		00000	0.000		0.003604					
	SCALE3	0.00	00000	0.000	000	0.00500.		_			
		-	CD.	LEU	306	6.638	11.502	3.989	1.00	61.20	
	MOTA	1	CB	LEU	306	7.381	10.684	6.231	1.00	61.47	
	MOTA	2	C		306	6.407	11.020	6.905	1.00	62.09	
20	MOTA	3	0	LEU	306	6.369	9.128	4.588		62.32	
	MOTA	4	N	LEU		7.232	10.330	4.754	1.00	61.30	
	MOTA	5	CA	LEU	306	8.609	10.605	6.730	1.00	60.52	
	MOTA	6	N	ALA	307	8.891	10.912	8.125	1.00	58.77	
	MOTA	7	CA	ALA	307	10.318	10.512	8.465	1.00	59.70	
25	MOTA	8	CB	ALA	307		12.393	8.429	1.00	57.51	
	MOTA	9	С	ALA	307	8.692	12.770	9.574	1.00	57.64	
	MOTA	10	0	ALA	307	8.451	13.228	7.400	1.00	55.82	
	MOTA	11	N	LEU	308	8.789		7.573	1.00	56.62	
	MOTA	12	CA	LEU	308	8.638	14.668	6.406	1.00	57.48	
30	MOTA	13	CB	LEU	308	9.298	15.402	5.948	1.00	59.17	
	ATOM	14	CG	LEU	308	10.637	14.822	4.569	1.00	60.38	
	MOTA	15	CD1	LEU	308	10.474		5.933	1.00	58.46	
	MOTA	16	CD2	LEU	308	11.694			1.00	56.51	
	MOTA	17	C	LEU	308	7.190		7.710	1.00	55.58	
35	MOTA	18	0	LEU	308	6.935		7.961		57.04	
	MOTA	19	N	SER	309	6.246		7.546	1.00	56.46	
	MOTA	20	CA	SER	309	4.828		7.657	1.00		
	MOTA	21	CB	SER	309	4.034		6.514	1.00	56.79	
	MOTA	22	OG	SER	309	4.071		6.588	1.00	57.23	
40	MOTA	23	C	SER	309	4.261		9.003	1.00	56.13	
	ATOM	24	0	SER	309	3.166		9.398	1.00	55.17	
	MOTA	25	N	LEU	310	5.016		9.706	1.00	54.31	
	MOTA	26	CA	LEU	310	4.591		11.004	1.00	53.55	
	MOTA	27	CB	LEU	310	5.651		11.582	1.00	54.40	
45	MOTA	28	CG	LEU	310	5.586		11.189	1.00	56.49	
	MOTA	29	CD1	LEU	310	5.530		9.676	1.00	57.06	
	ATOM	30	CD2	LEU	310	6.809		11.739	1.00	57.28	
	MOTA	31	С	LEU	310	4.33		12.003	1.00	53.18	
	MOTA	32	0	LEU	310	4.99	3 14.905	11.984	1.00	53.17	
50		33	N	THR	311	3.35				51.71	
50	MOTA	34	CA	THR	311	3.01				49.93	
	MOTA	35	CB	THR	311	1.52	7 14.554			48.96	
	MOTA	36	OG1		311	1.24	2 13.311	14.930		47.20	
	MOTA	37	CG2		311	0.66	6 14.688	13.027	1.00	50.99	
55		38	C	THR			5 14.201	15.145		48.84	
55	ATOM	39	0	THR					1.00	46.66	
	MOTA	40	N	ALA				16.141	1.00	48.76	
	MOTA	41	CA	ALA					1.00		
		42	CB	ALA					1.00		
60	MOTA (43	C	ALA					1.00	47.41	
00	MOTA (43	C		. ,						

5	MOTA	44	0	ALA	312	5.009	12.609	18.262	1.00	45.52
	MOTA	45	N	ASP	313	2.868	13.275	18.143	1.00	47.58
	MOTA	46	CA	ASP	313	2.367	12.032	18.714	1.00	47.63
	MOTA	47	CB	ASP	313	0.848	12.100	18.879	1.00	51.96
	MOTA	48	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
10	MOTA	49	OD1	ASP	313	1.314	13.234	20.929	1.00	56.38
	MOTA	50	OD2	ASP	313	-0.785	13.117	20.282	1.00	59.15
	MOTA	51	C	ASP	313	2.745	10.846	17.835	1.00	43.93
	MOTA	52	0	ASP	313	2.959	9.741	18.330	1.00	44.77
	MOTA	53	N	$_{ m GLN}$	314	2.826	11.081	16.531	1.00	44.52
15	ATOM	54	CA	GLN	314	3.182	10.028	15.588	1.00	44.73
	MOTA	55	CB	GLN	314	2.849	10.464	14.156	1.00	45.05
	MOTA	56	CG	${ t GLN}$	314	1.534	9.886	13.626	1.00	48.47
	MOTA	57	CD	GLN	314	0.982	10.646	12.428	1.00	50.37
	MOTA	58	OE1	GLN	314	1.649	11.515	11.856	1.00	49.38
20	MOTA	59	NE2	GLN	314	-0.248	10.318	12.043	1.00	51.74
	ATOM	60	С	GLN	314	4.673	9.722	15.707	1.00	43.26
	MOTA	61	0	GLN	314	5.100	8.580	15.555	1.00	43.93
	MOTA	62	N	MET	315	5.459	10.757	15.980	1.00	42.29
	MOTA	63	CA	MET	315	6.901	10.606	16.130	1.00	41.26
25	ATOM	64	CB	MET	315	7.565	11.985	16.224	1.00	42.43
	MOTA	65	CG	MET	315	9.082	11.939	16.356	1.00	42.34
	MOTA	66	SD	MET	315	9.906	11.190	14.925	1.00	46.22
	MOTA	67	CE	MET	315	9.547	12.408	13.680	1.00	37.32
	MOTA	68	С	\mathtt{MET}	315	7.218	9.791	17.379	1.00	38.89
30	MOTA	69	0	MET	315	8.002	8.841	17.335	1.00	40.02
	MOTA	70	N	VAL	316	6.599	10.165	18.491	1.00	37.65
	MOTA	71	CA	VAL	316	6.819	9.476	19.756	1.00	39.56
	ATOM	72	CB	VAL	316	6.023	10.136	20.897	1.00	39.22
	ATOM	73	CG1	VAL	316	6.245	9.373	22.192	1.00	44.43
35	MOTA	74	CG2	VAL	316	6.446	11.583	21.059	1.00	41.04
	ATOM	75	С	VAL	316	6.404	8.012	19.664	1.00	40.04
	MOTA	76	0	VAL	316	7.141	7.117	20.077	1.00	37.86
	MOTA	77	N	SER	317	5.215	7.767	19.127	1.00	41.90
4.0	MOTA	78	CA	SER	317	4.733	6.400	18.997	1.00	41.68
40	MOTA	79	CB	SER	317	3.311	6.402	18.415	1.00	43.85
	MOTA	80	OG	SER	317	3.225	5.631	17.230	1.00	49.38
	MOTA	81	C	SER	317	5.696		18.114		
	ATOM	82	0	SER	317	6.011	4.446	18.407		40.21
15	MOTA	83	N	ALA	318	6.182	6.220	17.043		38.35
45	ATOM	84	CA	ALA	318	7.114		16.153		36.96
	MOTA	85	CB	ALA	318	7.485		14.986	1.00	37.92
	MOTA	86	C	ALA	318	8.375		16.920	1.00 1.00	38.31
	MOTA	87	0	ALA	318	8.820	3.992	16.844		33.94
50	ATOM	88	N	LEU	319	8.938	6.089	17.664		36.92
50	MOTA	89	CA	LEU	319	10.161	5.854	18.438	1.00	38.56
	MOTA	90	CB	LEU	319	10.660	7.174	19.040	1.00	40.86
	MOTA	91	CG	LEU	319	11.136	8.264	18.071	1.00	41.25
	MOTA	92	CD1	LEU	319	11.714	9.440	18.857		
55	ATOM	93	CD2	LEU	319	12.182	7.693	17.140 19.549		42.61 38.33
22	ATOM	94	C	LEU	319	9.965	4.826			
	MOTA	95 06	0	LEU	319	10.779	3.916	19.729		33.91
	ATOM	96 07	N	LEU	320	8.879	4.982	20.297		37.39
	ATOM	97 08	CA	LEU	320	8.567	4.067	21.387		
60	MOTA	98	CB	LEU	320	7.239	4.467			
OU	ATOM	99 100	CG	LEU	320	7.236	5.582			
	MOTA	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96

								•		
5	ATOM	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
_	MOTA	102	C	LEU	320	8.466	2.642	20.843	1.00	41.11
	MOTA	103	Ō	LEU	320	8.971	1.697	21.443	1.00	41.87
	ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
	ATOM	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
10				ASP	321	6.669	1.372	17.860	1.00	48.39
10	ATOM	106	CB			5.206	1.318	18.255	1.00	52.39
	MOTA	107	CG	ASP	321			19.464	1.00	53.56
	ATOM	108	OD1	ASP	321	4.901	1.422			55.81
	ATOM	109	OD2	ASP	321	4.357	1.172	17.346	1.00	
	MOTA	110	C	ASP	321	8.911	0.565	18.568	1.00	44.37
15	MOTA	111	0	ASP	321	9.030	-0.661	18.533	1.00	44.67
	MOTA	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	MOTA	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
	MOTA	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
	MOTA	115	С	ALA	322	12.148	0.513	18.769	1.00	35.52
20	ATOM	116	0	ALA	322	13.219	-0.020	18.473	1.00	36.11
	ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	MOTA	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
	MOTA	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
	ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
25	ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
23	ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
		124	C	GLU	323	13.205	-0.978	21.110	1.00	38.01
	MOTA				323	12.425	-1.931	20.999	1.00	38.37
20	ATOM	125	0	GLU	323	14.527	-1.151	21.225	1.00	36.03
30	ATOM	126	N	PRO			-0.069	21.345	1.00	36.69
	ATOM	127	CD	PRO	324	15.522			1.00	36.42
	ATOM	128	CA	PRO	324	15.158	-2.474	21.240		
	MOTA	129	CB	PRÒ	324	16.633	-2.166	21.003	1.00	35.75
	MOTA	130	CG	PRO	324	16.811	-0.807	21.610	1.00	35.46
35	MOTA	131	С	PRO	324	14.940	-3.162	22.583	1.00	35.75
	ATOM	132	0	PRO	324	14.616	-2.517	23.580	1.00	34.97
	ATOM	133	N	PRO	325	15.134	-4.485	22.631	1.00	35.24
	MOTA	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
	MOTA	135	CA	PRO	325	14.942	-5.208	23.889	1.00	34.65
40	MOTA	136	CB	PRO	325	14.753	-6.652	23.439	1.00	35.83
	MOTA	137	CG	PRO	325	15.589	-6.743	22.200	1.00	34.88
	MOTA	138	С	PRO	325	16.132	-5.070	24.824		34.51
	MOTA	139	0	PRO	325	17.237	-4.723	24.399	1.00	
	ATOM	140	N	ILE	326	15.899	-5.322	26.106	1.00	
45	MOTA	141	CA	ILE	326	16.975	-5.265	27.075	1.00	35.02
	ATOM	142	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
	ATOM	143	CG2	ILE	326	17.557	-5.110	29.504	1.00	38.70
	MOTA	144	CG1	ILE	326	15.987	-3.431	28.466	1.00	40.48
	ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
50	ATOM	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
-	ATOM	147	Ō	ILE	326	16.875	-7.634	27.427		
	MOTA	148	N	LEU	327	18.840	-6.784	26.745		
	MOTA	149	CA	LEU	327	19.493	-8.083	26.716		
			CB	LEU	327	20.528	-8.135	25.587		
55	ATOM	150	CG	LEU	327	19.978	-7.800	24.196		
دد	ATOM	151			327	21.068	-7.800	23.139		
	ATOM	152	CD1	LEU						
	ATOM	153	CD2	LEU	327	18.775	-8.688	23.891		
	ATOM	154	С	LEU	327	20.156	-8.438	28.030		
~^	MOTA	155	0	LEU	327	20.393	-7.578	28.891		
60	MOTA	156	N	TYR	328	20.445	-9.725			
	MOTA	157	CA	TYR	328	21.087	-10.229	29.381	1.00	30.95

5	MOTA	158	CB	TYR	328		-11.520	29.842	1.00	33.38
	ATOM	159	CG	TYR	328		-11.272	30.686	1.00	33.05
	MOTA	160	CD1	TYR	328		-11.398	32.071	1.00	31.92
	MOTA	161	CE1	TYR	328	18.152	-11.114	32.864	1.00	36.01
	MOTA	162	CD2	TYR	328	17.996	-10.862	30.110	1.00	36.05
10	MOTA	163	CE2	TYR	328	16.880	-10.574	30.899	1.00	37.27
	MOTA	164	CZ	TYR	328	16.973	-10.702	32.274	1.00	37.66
	MOTA	165	OH	TYR	328	15.896	-10.397	33.071	1.00	44.66
	MOTA	166	С	TYR	328	22.529	-10.520	29.067	1.00	33.66
	ATOM	167	0	TYR	328	22.884	-10.744	27.910	1.00	34.78
15	ATOM	168	N	SER	329	23.359	-10.496	30.103	1.00	33.97
	MOTA	169	CA	SER	329	24.767	-10.800	29.962	1.00	37.29
	MOTA	170	CB	SER	329	25.526	-10.342	31.204	1.00	36.51
	ATOM	171	OG	SER	329	26.787	-10.965	31.282	1.00	37.13
	MOTA	172	С	SER	329	24.835	-12.317	29.832	1.00	40.43
20	MOTA	173	0	SER	329	23.980	-13.028	30.363	1.00	40.11
	ATOM	174	N	GLU	330	25.845	-12.811	29.128	1.00	41.40
	MOTA	175	CA	GLU	330	25.992	-14.242	28.928	1.00	47.43
	ATOM	176	CB	GLU	330	26.423	-14.524	27.484	1.00	48.64
	MOTA	177	CG	GLU	330	25.278	-14.870	26.542	1.00	50.20
25	MOTA	178	CD	GLU	330	25.765	-15.405	25.198	1.00	53.25
	ATOM	179	OE1	GLU	330	25.909	-16.640	25.062	1.00	53.27
	MOTA	180	OE2	GLU	330	26.004	-14.590	24.280	1.00	51.80
	MOTA	181	С	GLU	330	26.999	-14.852	29.893	1.00	49.67
	MOTA	182	0	GLU	330	28.207	-14.741	29.696	1.00	50.11
30	ATOM	183	N	TYR	331	26.498	-15.493	30.942	1.00	53.62
	ATOM	184	CA	TYR	331	27.373	-16.130	31.921	1.00	58.16
	MOTA	185	CB	TYR	331	28.092	-15.078	32.774	1.00	59.55
	ATOM	186	CG	TYR	331	27.239	-14.460	33.860	1.00	63.08
	MOTA	187	CD1	TYR	331	26.656	-13.205	33.682	1.00	64.50
35	MOTA	188	CE1	TYR	331	25.864	-12.630	34.676	1.00	65.99
	MOTA	189	CD2	TYR	331	27.010	-15.128	35.065	1.00	63.52
	MOTA	190	CE2	TYR	331	26.219	-14.563	36.066	1.00	65.60
	MOTA	191	CZ	TYR	331	25.648	-13.314	35.864	1.00	67.20
	MOTA	192	OH	TYR	331	24.855	-12.753	36.839	1.00	67.40
40	MOTA	193	С	TYR	331	26.603		32.823	1.00	59.05
	MOTA	194	0	TYR	331	25.393		33.002	1.00	59.22
	MOTA	195	N	ASP	332		-18.045	33.387		61.62
	MOTA	196	CA	ASP	332		-19.026	34.281		64.20
	MOTA	197	CB	ASP	332		-20.194	34.500		65.99
45	MOTA	198	CG	ASP	332		-21.516	34.648		68.11
	MOTA	199	OD1	ASP	332		-22.564	34.351		69.54
	MOTA	200	OD2	ASP	332		-21.505	35.060		67.40
	MOTA	201	С	ASP	332		-18.371	35.619		63.33
	MOTA	202	0	ASP	332		-18.073	36.406		63.90
50	MOTA	203	N	PRO	333		-18.148	35.896		
	MOTA	204	CD	PRO	333		-18.509	35.053		64.35
	MOTA	205	CA	PRO	333		7 -17.521	37.154		
	MOTA	206	CB	PRO	333	23.165		36.993		
	ATOM	207	CG	PRO	333	22.866		35.556		
55	ATOM	208	C	PRO	333	25.010		38.332		
	MOTA	209	0	PRO	333	25.129		39.468		
	MOTA	210	N	THR	334	25.160		38.037		
	MOTA	211	CA	THR	334	25.475		39.050		
	MOTA	212	CB	THR		24.929		38.645		
60	MOTA	213	OG1	THR		25.57		37.439		
	MOTA	214	CG2	THR	334	23.423	3 -22.012	38.411	1.00	67.57

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5	ATOM	215	С	THR	334	26.982	-20 004	20 260	7 00	
•	ATOM	216	0	THR	334		-20.804	39.269	1.00	65.67
	ATOM	217				27.432	-21.323	40.289	1.00	64.77
			И	ARG	335	27.759	-20.308	38.313	1.00	65.65
	ATOM	218	CA	ARG	335	29.214	-20.360	38.421	1.00	66.60
10	ATOM	219	CB	ARG	335	29.835	-20.500	37.030	1.00	66.74
10	ATOM	220	С	ARG	335	29.757	-19.113	39.123	1.00	67.09
	ATOM	221	0	ARG	335	29.100	-18.071	39.148	1.00	67.31
	ATOM	222	N	PRO	336	30.968	-19.207	39.702	1.00	67.62
	MOTA	223	CD	PRO	336	31.820	-20.408	39.713	1.00	67.30
	MOTA	224	CA	PRO	336	31.601	-18.086	40.410	1.00	67.42
15	ATOM	225	CB	PRO	336	32.982	-18.621	40.783	1.00	66.43
	ATOM	226	CG	PRO	336	32.829	-20.097	40.779	1.00	67.52
	MOTA	227	С	PRO	336	31.701	-16.828	39.561	1.00	
	MOTA	228	0	PRO	336	31.996	-16.895	38.371		68.26
	ATOM	229	N	PHE	337	31.460	-15.681		1.00	69.04
20	ATOM	230	CA	PHE	337	31.529	-14.408	40.183	1.00	69.49
- +	MOTA	231	CB	PHE	337			39.480	1.00	71.39
	MOTA	232	CG	PHE		30.818	-13.323	40.294	1.00	72.31
	ATOM	233	CD1		337	31.219	-11.924	39.921	1.00	73.21
				PHE	337	30.632	-11.287	38.833	1.00	72.82
25	ATOM	234	CD2	PHE	337	32.191	-11.245	40.653	1.00	73.43
د ک	ATOM	235	CE1	PHE	337	31.006	-9.993	38.479	1.00	73.28
	ATOM	236	CE2	PHE	337	32.573	-9.950	40.306	1.00	73.00
	MOTA	237	CZ	PHE	337	31.980	-9.323	39.217	1.00	72.90
	MOTA	238	С	PHE	337	32.985	-14.013	39.245	1.00	71.38
20	ATOM	239	0	PHE	337	33.336	-13.487	38.189	1.00	71.56
30	ATOM	240	N	SER	338	33.825	-14.273	40.241	1.00	71.53
	ATOM	241	CA	SER	338	35.248	-13.947	40.172	1.00	70.98
	MOTA	242	CB	SER	338	35.957	-14.487	41.414	1.00	70.43
	MOTA	243	OG	SER	338	35.547	-15.818	41.679	1.00	69.59
	MOTA	244	С	SER	338	35.931	-14.504	38.924	1.00	71.20
35	MOTA	245	0	SER	338	36.951	-13.972	38.475	1.00	71.35
	MOTA	246	N	GLU	339	35.368	-15.573	38.369	1.00	70.20
	MOTA	247	CA	GLU	339	35.930	-16.215	37.183	1.00	69.48
	MOTA	248	CB	GLU	339	35.279	-17.585	36.971	1.00	71.07
	MOTA	249	CG	GLU	339	35.996	-18.740	37.656	1.00	72.60
40	ATOM	250	CD	GLU	339	35.382	-20.089	37.318	1.00	74.26
	MOTA	251	OE1	GLU	339	34.786	-20.220	36.227	1.00	
	MOTA	252	OE2	GLU	339		-21.020	38.144		73.51
	ATOM	253	C	GLU	339		-15.385	35.910		76.44
	MOTA	254	Ö	GLU	339	36.722			1.00	68.15
45	ATOM	255	N	ALA	340	34.562		35.144	1.00	68.99
	MOTA	256	CA	ALA	340	34.246		35.694	1.00	64.41
	ATOM	257	CB	ALA	340	32.767		34.507	1.00	60.69
	ATOM	258	C	ALA				34.523	1.00	61.17
	ATOM	259	0		340	35.096	-12.824	34.326	1.00	57.00
50	ATOM			ALA	340	35.634	-12.270	35.287	1.00	57.46
50		260	N	SER	341	35.215	-12.388	33.076	1.00	52.15
	ATOM	261	CA	SER	341	35.972	-11.188	32.736	1.00	46.53
	ATOM	262	CB	SER	341	36.839	-11.439	31.497	1.00	48.64
	ATOM	263	OG	SER	341	37.184	-10.226	30.846	1.00	46.48
	ATOM	264	С	SER	341	34.957	-10.087	32.444	1.00	43.52
55	ATOM	265	0	SER	341	34.090	-10.248	31.589	1.00	39.92
	ATOM	266	N	MET	342	35.052	-8.978	33.166	1.00	41.24
	MOTA	267	CA	MET	342	34.121	-7.875	32.960	1.00	42.46
	ATOM	268	CB	MET	342	34.449	-6.723	33.912	1.00	45.61
	ATOM	269	CG	MET	342	33.228	-6.089	34.560	1.00	52.39
60	ATOM	270	SD	MET	342	31.791	-7.201	34.631	1.00	57.92
	MOTA	271	CE	MET	342	31.999	-7.881	36.239	1.00	56.18
								30.237	1.00	30.10

5	ATOM	272	C	MET	342	34.124	-7.365	31.516	1.00	40.22
	MOTA	273	0	MET	342	33.063	-7.121	30.938	1.00	39.23
	MOTA	274	N	MET	343	35.307	-7.204	30.930	1.00	38.72
	MOTA	275	CA	MET	343	35.395	-6.708	29.558	1.00	38.50
	MOTA	276	CB	MET	343	36.838	-6.318	29.216	1.00	41.15
10	MOTA	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	ATOM	278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
	ATOM	279	CE	MET	343	36.113	-3.358	28.987	1.00	40.45
	MOTA	280	С	MET	343	34.880	-7.741	28.561	1.00	35.36
	MOTA	281	0	MET	343	34.368	-7.384	27.501	1.00	35.51
15	MOTA	282	N	$\operatorname{\mathbf{GLY}}$	344	35.017	-9.020	28.902	1.00	35.53
	MOTA	283	CA	\mathtt{GLY}	344	34.533	-10.072	28.024	1.00	33.41
	MOTA	284	C	GLY	344	33.015	-10.063	28.047	1.00	31.74
	ATOM	285	0	GLY	344	32.359	-10.233	27.019	1.00	29.58
	ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
20	ATOM	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	MOTA	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
	ATOM	. 289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
	ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
	ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
25	MOTA	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
20	ATOM	293	Õ	LEU	345	29.479	-8.757	27.868	1.00	30.29
	MOTA	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
	MOTA	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
	MOTA	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
30	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
50	ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
	MOTA	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
	ATOM	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
	ATOM	301	0	LEU	346	29.869	-5.765	25.955	1.00	29.13
35	ATOM	302	N	THR	347	31.839	-6.816	26.212	1.00	30.47
33	ATOM	303	CA	THR	347	32.086	-6.911	24.781	1.00	30.93
	MOTA	304	CB	THR	347	33.472	-7.501	24.497	1.00	29.97
	ATOM	305	OG1	THR	347	34.481	-6.604	24.982	1.00	35.40
	ATOM	306	CG2	THR	347	33.666	-7.707	23.004	1.00	33.58
40	ATOM	307	C	THR	347	31.036	-7.804	24.122	1.00	31.97
	ATOM	308	0	THR	347	30.516	-7.486	23.049	1.00	30.75
	ATOM	309	И	ASN	348	30.737		24.768	1.00	29.31
	ATOM	310	CA	ASN	348	29.757	-9.868	24.700	1.00	32.63
	MOTA	311	CB	ASN	348		-11.161	25.065	1.00	31.64
45	ATOM	312	CG	ASN	348	28.646		24.662	1.00	39.14
73	ATOM	313	OD1	ASN	348	27.549		25.220	1.00	41.91
	ATOM	314	ND2	ASN	348	28.920		23.220	1.00	42.05
	ATOM	315	C	ASN	348	28.361	-9.251	24.262	1.00	29.02
	ATOM	316								
50			O N	ASN	348	27.558	-9.477	23.353	1.00	32.76
30	MOTA	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
	MOTA	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58
	ATOM	319	CB	LEU	349	26.650	-7.148	26.795	1.00	26.56
	ATOM	320	CG	LEU	349	25.376	-6.328	27.050	1.00	33.67
55	ATOM	321	CD1	LEU	349	24.140	-7.199	26.840	1.00	28.82
55	ATOM	322	CD2	LEU	349	25.392	-5.779	28.471	1.00	33.11
	MOTA	323	C	LEU	349	26.638	-6.762	24.319	1.00	28.07
	ATOM	324	0	LEU	349	25.616	-6.703	23.629	1.00	25.22
	ATOM	325	N	ALA	350	27.675	-5.941	24.157	1.00	28.50
~	ATOM	326	CA	ALA	350	27.668	-4.886	23.148	1.00	28.46
60	MOTA	327	CB	ALA	350	28.972	-4.094	23.209	1.00	28.12
	ATOM	328	С	ALA	350	27.468	-5.461	21.750	1.00	28.75

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5	MOTA	329	0	ALA	350	26.649	-4.958	20.983	1.00	30.90
	MOTA	330	N	ASP	351	28.213	-6.509	21.420	1.00	27.20
	MOTA	331	CA	ASP	351	28.093	-7.143	20.112	1.00	29.75
	MOTA	332	CB	ASP	351	29.036	-8.345	20.010	1.00	34.16
	MOTA	333	CG	ASP	351	30.498	-7.940	19.978	1.00	37.50
10	MOTA	334	OD1	ASP	351	31.354	-8.831	20.148	1.00	37.55
	MOTA	335	OD2	ASP	351	30.789	-6.738	19.784	1.00	35.50
	MOTA	336	C	ASP	351	26.661	-7.600	19.813	1.00	30.52
	MOTA	337	0	ASP	351	26.193	-7.458	18.687	1.00	27.77
	MOTA	338	N	ARG	352	25.968	-8.150	20.811	1.00	27.18
15	MOTA	339	CA	ARG	352	24.593	-8.602	20.605	1.00	26.21
	MOTA	340	CB	ARG	352	24.148	-9.534	21.752	1.00	26.52
	MOTA	341	CG	ARG	352	24.567	-10.991	21.532	1.00	31.03
	MOTA	342	CD	ARG	352	24.128	-11.911	22.666	1.00	29.80
	MOTA	343	NE	ARG	352	24.898	-11.675	23.879	1.00	30.44
20	MOTA	344	CZ	ARG	352	24.364	-11.363	25.054	1.00	31.68
	MOTA	345	NH1	ARG	352	23.050	-11.251	25.177	1.00	31.18
	MOTA	346	NH2	ARG	352	25.144	-11.148	26.104	1.00	32.03
	MOTA	347	C	ARG	352	23.642	-7.411	20.502	1.00	27.16
	ATOM	348	0	ARG	352	22.702	-7.426	19.708	1.00	26.65
25	MOTA	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
	MOTA	350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
	MOTA	351	CB	GLU	353	23.461	-4.204	22.365	1.00	24.91
	MOTA	352	CG	GLU	353	23.147	-4.669	23.771	1.00	27.93
	ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
30	MOTA	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
	MOTA	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
	MOTA	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
	MOTA	357	0	GLU	353	22.169	-3.826	19.467	1.00	28.71
	MOTA	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
35	MOTA	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
	MOTA	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
	MOTA	361	CG	LEU	354	26.372	-3.257	16.351	1.00	29.24
	MOTA	362	CD1	LEU	354	26.243	-1.774	16.722	1.00	26.59
40	MOTA	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
40	MOTA	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
	ATOM	365	0	LEU	354	23.074	-3.475	16.152	1.00	24.00
	MOTA	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
	MOTA	367	CA	VAL	355	22.386	-6.125	15.844	1.00	29.45
45	MOTA	368	CB	VAL	355	22.259	-7.655	15.975	1.00	31.76
43	MOTA	369	CG1	VAL	355	21.423	-8.205	14.834	1.00	33.55
	ATOM	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	31.36
	ATOM	371	C	VAL	355	21.020	-5.499	16.035	1.00	27.71
	MOTA	372	0	VAL	355	20.382	-5.039	15.080	1.00	29.61
50	MOTA	373	N	HIS	356	20.580	-5.473	17.288	1.00	27.76
50	ATOM	374	CA	HIS	356	19.291	-4.906	17.627	1.00	28.35
	MOTA	375	CB	HIS	356	18.936	-5.231	19.079	1.00	31.12
	MOTA	376	CG	HIS	356	18.602	-6.675	19.307	1.00	35.93
	MOTA	377	CD2	HIS	356	19.352	-7.700	19.779	1.00	33.95
55	MOTA	378	ND1	HIS	356	17.363	-7.208	19.018	1.00	36.62
55	MOTA	379	CE1	HIS	356 356	17.364	-8.499	19.304	1.00	33.33
	MOTA	380	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
	MOTA	381	C	HIS	356 356	19.300	-3.398	17.412	1.00	28.25
	MOTA	382	0	HIS	356	18.272	-2.812	17.100	1.00	28.99
60	ATOM	383	N	MET	357	20.457	-2.765	17.574	1.00	25.31
00	ATOM	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	MOTA	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61

5	MOTA	386	CG	MET	357	22.011	0.736	17.699		24.66
	ATOM	387	SD	MET	357	23.732	1.290	17.859		27.30 23.62
	MOTA	388	CE	MET	357	24.140	0.672	19.514		24.83
	MOTA	389	C	MET	357	20.256	-1.011	15.898		24.03
	MOTA	390	0	MET	357	19.619	-0.003	15.569	1.00	26.76
10	MOTA	391	N	ILE	358	20.757	-1.874	15.020		30.33
	MOTA	392	CA	ILE	358	20.553	-1.721	13.576	1.00	33.86
	MOTA	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.68
	MOTA	394	CG2	ILE	358	20.759	-2.860	11.334 12.874	1.00	36.89
	MOTA	395	CG1	ILE	358	22.728	-2.799	12.674	1.00	39.10
15	MOTA	396	CD1	ILE	358	23.299	-1.469	13.310	1.00	32.20
	MOTA	397	C	ILE	358	19.055	-1.721 -0.817	12.662	1.00	32.02
	MOTA	398	0	ILE	358	18.519		13.814	1.00	33.12
	MOTA	399	N	ASN	359	18.379	-2.748 -2.861	13.614	1.00	33.35
	MOTA	400	CA	ASN	359	16.945	-4.101	14.363	1.00	37.59
20	MOTA	401	CB	ASN	359	16.434	-5.374	13.627	1.00	44.38
	MOTA	402	CG	ASN	359	16.739 17.045	-5.329	12.437	1.00	47.35
	MOTA	403	OD1	ASN	359	16.673	-6.508	14.320	1.00	42.48
	MOTA	404	ND2	ASN	359 359	16.073	-1.634	14.149	1.00	32.74
25	MOTA	405	C	ASN ASN	35 <i>9</i> 359	15.261	-1.163	13.530	1.00	31.39
25	ATOM	406	0	TRP	360	16.706	-1.104	15.264	1.00	27.92
	MOTA	407	N CA	TRP	360	16.102	0.087	15.842	1.00	29.47
	MOTA	408 409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
	MOTA	410	CG	TRP	360	16.522	1.747	17.707	1.00.	30.40
30	MOTA MOTA	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
30	ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
	MOTA	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
	MOTA	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
35	MOTA	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
	MOTA	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
	MOTA	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
	MOTA	419	С	TRP	360	16.312	1.296	14.926	1.00	27.90
	MOTA	420	0	TRP	360	15.360	2.002	14.581	1.00	28.83
40	MOTA	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
	MOTA	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
	MOTA	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
	MOTA	424	С	ALA	361	17.006	2.685	12.403		31.08
	MOTA	425	0	ALA	361	16.531	3.746	12.011		31.30
45	MOTA	426	N	LYS	362	16.795	1.526	11.783		30.93 34.15
	MOTA	427	CA	LYS	362	15.981	1.443	10.581		
	MOTA	428	CB	LYS	362	16.012	0.016	10.023		
	ATOM	429	CG	LYS	362	17.252	-0.281	9.198 9.136		
	MOTA	430	CD	LYS	362	17.547				
50	MOTA	431	CE	LYS	362	18.852				
	MOTA	432	ΝZ	LYS	362	19.178				
	MOTA	433	C	LYS		14.545				
	ATOM	434	0	LYS		13.821				
~ ~	MOTA	435		ARG		14.134				
55		436		ARG		12.770 12.178				
	MOTA	437		ARG		12.178				_
	MOTA	438		ARG		11.468				_
	MOTA	439		ARG		10.161				
<i>د</i> ۸	MOTA	440		ARG ARG		9.314				
60		441				9.642				
	MOTA	442	NHI	. ARG	303	J. 042	2.307			

5	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
	ATOM	444	С	ARG	363	12.654	3.743	12.943	1.00	37.40
	MOTA	445	0	ARG	363	11.567	4.199	13.303	1.00	38.22
	ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
	ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
10	MOTA	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
	ATOM	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
	ATOM	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30
	MOTA	451	C	VAL	364	13.360	6.591	12.171	1.00	33.19
	MOTA	452	0	VAL	364	14.028	6.531	11.146	1.00	33.04
15	MOTA	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
	ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
	MOTA	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
	ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
20	MOTA	458	С	PRO	365	12.756	8.878	10.321	1.00	37.19
	MOTA	459	0	PRO	365	13.430	9.726	10.907	1.00	40.29
	MOTA	460	N	GLY	366	12.878	8.624	9.023	1.00	34.78
	MOTA	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
	MOTA	462	С	\mathtt{GLY}	366	15.168	8.722	8.00.7	1.00	34.26
25	MOTA	463	0	GLY	366	15.858	9.035	7.034	1.00	37.15
	ATOM	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
	ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	MOTA	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
	MOTA	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60
30	MOTA	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
	MOTA	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
	MOTA	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
	MOTA	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
35	MOTA	473	С	PHE	367	17.033	6.333	7.524	1.00	31.46
	MOTA	474	0	PHE	367	18.073	6.405	6.883	1.00	32.30
	ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
	MOTA	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
	MOTA	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
40	MOTA	478	CG1	VAL	368	15.543	2.447	6.843	1.00	41.48
	MOTA	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
	MOTA	480	С	VAL	368	15.965	5.523			40.06
	MOTA .	481	0	VAL	368	16.156	4.992	3.579		41.66
	MOTA	482	N	ASP	369	15.608	6.798			
45	ATOM	483	CA	ASP	369	15.465	7.646			
	MOTA	484	CB	ASP	369	14.700	8.929			
	MOTA	485	CG	ASP	369	13.254	8.671		1.00	45.59
	MOTA	486	OD1	ASP	369	12.686	7.672	3.806		46.34
	MOTA	487	OD2	ASP	369	12.681	9.472	5.074		49.13
50	MOTA	488	C	ASP	369	16.855	8.010	3.136		34.91
	MOTA	489	0	ASP	369	17.038	8.431	1.995		34.25
	ATOM	490	N	LEU	370	17.838	7.841	4.016		31.76
	MOTA	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
	ATOM	492	CB	LEU	370	20.020	8.339	5.003		
55	ATOM	493	CG	LEU	370	19.523	9.395	6.000		
	ATOM	494	CD1	LEU	370	20.315	9.275	7.299		
	ATOM	495	CD2	LEU	370	19.693	10.792	5.404	1.00	
	ATOM	496	С	LEU	370	19.884	7.043	2.893	1.00	
	ATOM	497	0	LEU	370	19.341	5.943	2.784	1.00	31.78
60	MOTA	498	N	THR	371	21.052	7.333	2.331	1.00	28.86
	MOTA	499	CA	THR	371	21.793	6.336	1.569	1.00	32.90

						22 270	6.944	0.818	1.00 3	33.44
5	MOTA	500	CB	THR	371	22.979 23.880	7.523			34.59
	MOTA	501	OG1	THR	371	22.514				32.63
	MOTA	502	CG2	THR	371 371	22.373	5.315	-		35.31
	MOTA	503	C	THR		22.536	5.591			31.27
	MOTA	504	0	THR	371 372	22.702	4.141			34.34
10	MOTA	505	N	LEU	372	23.273	3.073	2.822		35.46
	MOTA	506	CA	LEU	372 372	23.273	1.841	1.944		37.73
	MOTA	507	CB	LEU	372	24.362	0.704	2.515		42.43
	MOTA	508	CG	LEU	372	23.690	0.145	3.757		45.60
	MOTA	509	CD1	LEU	372	24.534	-0.383	1.455		44.29
15	MOTA	510	CD2	LEU	372	24.587	3.548	3.444	1.00	36.95
	MOTA	511	C	LEU LEU	372	24.813	3.374	4.643	1.00	35.57
	MOTA	512	0	HIS	373	25.442	4.159	2.627	1.00	35.68
	MOTA	513	N	HIS	373	26.729	4.656	3.099	1.00	36.60
••	MOTA	514	CA	HIS	373	27.506	5.282	1.935	1.00	44.01
20	MOTA	515	CB. CG	HIS	373	28.538	6.280	2.360	1.00	50.69
	MOTA	516	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
	MOTA	517	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
	MOTA	518 510	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
25	MOTA	519 520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
25	MOTA MOTA	521	C	HIS	373	26.575	5.669	4.244	1.00	36.22
	ATOM	521	0	HIS	373	27.350	5.650	5.201	1.00	33.05
	ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
	MOTA	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
30	MOTA	525	CB	ASP	374	24.354	8.603	4.713	1.00	30.12
50	ATOM	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
	MOTA	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
	MOTA	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
	MOTA	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
35	ATOM	530	0	ASP	374	25.152	7.275	7.587	1.00	27.04
	MOTA	53 1	N	GLN	375	23.944	5.877	6.309	1.00	25.71
	MOTA	532	CA	${ t GLN}$	375	23.403	5.157	7.454	1.00	26.68
	MOTA	533	CB	${\tt GLN}$	375	22.424	4.077	6.993	1.00	29.70
	MOTA	534	CG	GLN	375	21.101	4.616	6.484	1.00	29.16 35.87
40	MOTA	535	CD	${\tt GLN}$	375	20.219	3.514	5.940	1.00	30.97
	MOTA	536	OE1	${ t GLN}$	375	20.155	2.426	6.510	1.00	34.51
	MOTA	537	NE2	${ t GLN}$. 375	19.541	3.785	4.827		25.51
	MOTA	538		GLN		24.556	4.502	8.214 9.442		28.14
	MOTA	539		GLN		24.585	4.513	7.475		
45	MOTA	540		VAL		25.504	3.938	8.071		
	ATOM	541		VAL		26.659	3.281	7.003		
	MOTA	542		VAL		27.531	2.597 2.071	7.635		
	MOTA	543				28.812 26.745		6.341		
	MOTA	544					4.285	8.821		
50		545		LAV		27.526	4.029	9.948		
	MOTA	546		VAL		27.953		8.191		
	MOTA	547		HIS		27.785		8.814		
	MOTA	548		HIS		28.602				
	MOTA	549		HIS		28.792				
55		550								
	MOTA	551								
	MOTA	552								
	MOTA	553								
	MOTA	554								
60		555		HIS						
	MOTA	556	6 0	HIS	s 377	20.0//	,.102			

5	ATOM	557	N	LEU	378	26.678	7.206	10.107	1.00	24.58
	atom	558	CA	LEU	378	26.015	7.695	11.315		
	MOTA	559	CB	ĻEU	378	24.542	8.001	11.027	-	-
	ATOM	560	CG	LEU	378	24.291	9.180	10.073		
	MOTA	561	CD1	LEU	378	22.778	9.353	9.869		
10	MOTA	562	CD2		378	24.911	10.458			
	MOTA	563	С	LEU	378	26.120		10.642	-	=
	MOTA	564	Ō	LEU	378		6.695	12.459		
	ATOM	565	N	LEU	379	26.379	7.075	13.605		
	ATOM	566	CA	LEU		25.919	5.414	12.153		
15	ATOM	567	CB		379	26.000	4.388	13.182		
	ATOM	568		LEU	379	25.401	3.073	12.667	1.00	28.53
	ATOM		CG	LEU	379	23.875	3.023	12.845	1.00	30.29
		569	CD1	LEU	379	23.248	1.943	11.963	1.00	
	ATOM	570	CD2	LEU	379	23.563	2.759	14.312	1.00	
20	ATOM	571	С	LEU	379	27.430	4.176	13.670	1.00	
20	MOTA	572	0	LEU	379	27.653	3.979	14.866		
	MOTA	573	N	GLU	380	28.402	4.236	12.762	1.00	
	MOTA	574	CA	GLU	380	29.786	4.054	13.173	1.00	27.58
	ATOM	575	CB	GLU	380	30.730	4.036	11.968	1.00	30.36
	MOTA	576	CG	GLU	380	32.172	3.785	12.380	1.00	
25	ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	
	MOTA	578	OE1	GLU	380	32.869	4.048	10.120		45.23
	MOTA	579	OE2	GLU	380	34.004	2.646	11.386	1.00	42.99
	ATOM	580	С	GLU	380	30.218	5.159		1.00	45.79
	MOTA	581	0	GLU	380	31.056	4.937	14.133	1.00	27.50
30	MOTA	582	N	ACYS		29.637	6.339	15.010	1.00	
	MOTA	583	N	BCYS		29.645		13.965	0.75	24.89
	MOTA	584	CA	ACYS		29.969	6.352	13.980	0.25	25.79
	ATOM	585	CA	BCYS		29.993	7.466	14.826	0.75	24.12
	ATOM	586	CB	ACYS	381		7.481	14.847	0.25	24.8 <i>6</i>
35	MOTA	587	CB	BCYS	381	29.621	8.781	14.122	0.75	25.96
	ATOM	588	SG	ACYS	381	29.766	8.814	14.115	0.25	25.62
	ATOM	589	SG	BCYS	381	30.698	9.192	12.732	0.75	31.63
	ATOM	590	C	ACYS		30.227	10.312	15.059	0.25	25.40
	ATOM	591	C	BCYS	381	29.237	7.422	16.162	0.75	22.07
40	ATOM	592	0		381	29.211	7.498	16.159	0.25	23.97
	ATOM	593	0	ACYS	381	29.812	7.730	17.206	0.75	21.97
	ATOM	594	И	BCYS	381	29.724	7.940	17.187	0.25	23.99
	ATOM	595		ALA	382	27.974	7.012	16.128	1.00	23.41
	ATOM	596	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
45	ATOM	597	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
	ATOM		C	ALA	382	26.913	5.755	18.131	1.00	25.39
	ATOM	598	0	ALA	382	26.374	5.837	19.234	1.00	23.09
		599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
	ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
50	ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
50	MOTA	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
	ATOM	603	CD2	TRP	383	29.797	1.347	18.803	1.00	27.31
	MOTA	604	CE2	TRP	383	31.182	1.484	18.579	1.00	28.24
	MOTA	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
	ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	
55	ATOM	607	NE1	TRP	383	31.342	2.239	17.446	1.00	24.58
	MOTA	608	CZ2	TRP	383	32.133	0.909	19.420		27.35
	ATOM	609	CZ3	TRP	383	30.305	0.039		1.00	28.76
	ATOM	610	CH2	TRP	383	31.674	0.039	20.745		`28.09
	ATOM	611	C	TRP	383	27.356		20.496	1.00	29.77
60	ATOM	612	0	TRP	383	26.526	3.309	19.802	1.00	23.54
	ATOM	613	N	LEU	384	28.542	2.866	20.584	1.00	22.90
		_			J J 4	20.342	3.765	20.211	1.00	20.37

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5	ATOM	614	CA	LEU	384	28.864	3.713	21.640	1.00	22 41
	ATOM	615	CB	LEU	384	30.369	3.890	21.883	1.00	22.41
	ATOM	616	CG	LEU	384	30.824	3.645	23.336	1.00	24.98
	MOTA	617	CD1	LEU	384	30.273	2.305	23.336		27.33
	MOTA	618	CD2	LEU	384	32.336	3.648		1.00	29.71
10	ATOM	619	C	LEU	384	28.075	4.732	23.398	1.00	26.07
	ATOM	620	Ö	LEU	384	27.706		22.453	1.00	19.44
	ATOM	621	N	GLU	385	27.708	4.458	23.595	1.00	23.24
	ATOM	622	CA	GLU	385		5.909	21.885	1.00	20.80
	ATOM	623	CB	GLU	385	27.011	6.895	22.612	1.00	21.32
15	ATOM	624	CG	GLU		26.861	8.177	21.797	1.00	21.91
	MOTA	625	CD	GLU	385	28.115	9.020	21.705	1.00	21.61
	MOTA	626	OE1	GLU	385	27.882	10.256	20.860	1.00	29.53
	ATOM	625	OE2		385	27.374	11.256	21.401	1.00	30.54
	MOTA	628		GLU	385	28.188	10.219	19.658	1.00	29.97
20	ATOM		C	GLU	385	25.616	6.292	22.836	1.00	22.26
20	ATOM	629	0	GLU	385	25.022	6.438	23.902	1.00	22.26
		630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
	ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
	ATOM	632	,CB	ILE	386	23.328	4.455	20.498	1.00	22.88
25	ATOM	633	CG2	ILE	386	22.009	3.647	20.618	1.00	23.85
23	MOTA	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
	MOTA	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
	ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
	ATOM	637	0	ILE	386	22.823	3.818	23.746	1.00	24.75
20	ATOM	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
30	MOTA	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
	MOTA	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
	ATOM	641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
	ATOM	642	CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
25	ATOM	643	CD2	LEU	387	24.791	-0.631	22.652	1.00	26.29
35	ATOM	644	C	LEU	387	24.944	2.660	25.438	1.00	26.22
	MOTA	645	0	LEU	387	24.287	2.204	26.386	1.00	23.55
	MOTA	646	N	MET	388	25.751	3.713	25.554	1.00	23.92
	ATOM	647	CA	MET	388	25.924	4.385	26.835	1.00	24.26
40	ATOM	648	CB	MET	388	27.088	5.378	26.761	1.00	23.87
40	MOTA	649	CG	MET	388	28.440	4.722	26.743	1.00	24.08
	ATOM	650	SD	MET	388	29.726	5.992	26.736	1.00	27.70
	MOTA	651	CE	MET	388	31.139	5.041	27.078	1.00	21.74
	ATOM	652	C	MET	388	24.660	5.094	27.321	1.00	23.33
15	ATOM	653	0	MET	388	24.341	5.026	28.505	1.00	25.58
45	ATOM	654	N	ILE	389	23.935	5.775	26.436	1.00	24.62
	MOTA	655	CA	ILE	389	22.729	6.440	26.905	1.00	24.03
	ATOM	656	CB	ILE	389	22.132	7.439	25.852	1.00	27.01
	ATOM	657	CG2	ILE	389	21.413	6.705	24.706	1.00	23.98
50	ATOM	658	CG1	ILE	389	21.185	8.402	26.584	1.00	25.49
50	ATOM	659	CD1	ILE	389	20.431	9.383	25.683	1.00	25.45
	MOTA	660	C	ILE	389	21.694	5.401	27.349	1.00	26.54
	ATOM	661	0	ILE	389	20.938	5.631	28.294	1.00	22.58
	MOTA	662	N	\mathtt{GLY}	390	21.679	4.247	26.687	1.00	27.14
~ ~	MOTA	663	CA	GLY	390	20.753	3.201	27.090	1.00	28.42
55	MOTA	664	C	GLY	390	21.133	2.719	28.482	1.00	29.67
	MOTA	665	0	GLY	390	20.275	2.521	29.348	1.00	29.21
	MOTA	666	N	LEU	391	22.433	2.547	28.699	1.00	26.06
	MOTA	667	CA	LEU	391	22.955	2.091	29.983	1.00	29.23
	MOTA	668	CB	LEU	391	24.476	1.937	29.899	1.00	28.37
60	ATOM	669	CG	LEU	391	25.206	1.656	31.210	1.00	30.81
	ATOM	670	CD1	LEU	391	24.717	0.332	31.793	1.00	25.73
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						26.709	1.619	30.958 1	.00 25	.25
5	MOTA	671	CD2			26.703	3.070			.84
	MOTA	672	C				2.669	32.186 1	.00 29	.19
	ATOM	673	0			22.156	4.355			.91
	MOTA	674	N			22.817				.86
	MOTA	675	CA	VAL	392	22.506	5.369			.08
10	ATOM	676	CB	VAL	392	22.923	6.770			.32
10	ATOM	677	CG1	VAL	392	22.329	7.854			3.52
	ATOM	678	CG2	VAL	392	24.442	6.870			
		679	C	VAL	392	21.013	5.327	— · —		3.42
	MOTA	680	0	VAL	392	20.621	5.345	-		38
	ATOM		N	TRP	393	20.191	5.241	-		3.23
15	MOTA	681	CA	TRP	393	18.732	5.186	•	-	9.70
	MOTA	682		TRP	393	18.066	5.046	29.906		0.09
	ATOM	683	CB	TRP	393	16.605	4.670	29.953		3.50
	MOTA	684	CG		393	15.516	5.499	30.369		1.76
	MOTA	685	CD2	TRP		14.336	4.725	30.264		8.11
20	ATOM	686	CE2	TRP	393	15.419	6.821	30.824	1.00 3	2.56
	MOTA	687	CE3	TRP	393		3.459	29.618	1.00 3	4.31
	MOTA	688	CD1	TRP	393	16.057	3.486	29.801		4.36
	ATOM	689	NEl	TRP	393	14.696		30.597		7.93
	MOTA	690	CZ2	TRP	393	13.073	5.233	31.155		5.24
25	MOTA	691	CZ3	TRP	393	14.162	7.326	31.133		37.77
20	ATOM	692	CH2	TRP	393	13.007	6.531			32.07
	MOTA	693	С	TRP	393	18.256	4.051	32.191		32.12
	ATOM	694	0	TRP	393	17.460	4.275	33.109		31.90
	MOTA	695	N	ARG	394	18.738	2.837	31.957		36.63
30	ATOM	696	CA	ARG	394	18.288	1.729	32.787		36.41
30	MOTA	697	CB	ARG	394	18.492	0.389	32.065		36.50
		698		ARG	394	19.914	0.009			
	MOTA	699		ARG	394	19.929	-1.132			36.34
	ATOM	700		ARG	394	21.282	-1.561			33.97
2 ~	MOTA	700		ARG	394	21.864	-1.350	29.239		31.61
35	MOTA				394	21.208	-0.715			32.42
	ATOM	702			394	23.098	-1.784	29.022	1.00	29.81
	MOTA	703		ARG	394	18.911	1.697	34.180	1.00	36.69
	MOTA	704		ARG	394	18.445	0.966	35.048	1.00	37.07
	MOTA	705		SER		19.954	2.492		1.00	33.63
40		706		SER		20.603	2.564		1.00	35.69
	MOTA	70				22.112	2.784		1.00	32.94
	ATOM	70		SER		22.696	1.81			32.37
	MOTA	70:		SER		20.010				36.44
	MOTA	71		SER		20.389				38.68
45	5 ATOM	71		SER		19.076				36.46
	MOTA	71		MET						43.08
	MOTA	71				18.431				43.87
	MOTA	71				17.275		_		46.18
	MOTA	71	5 CG			17.481				49.58
5	MOTA 0	71	.6 SD			15.962				53.58
•	MOTA	71	.7 CE	ME		14.988				46.18
	ATOM	71		ME'	r 396					46.34
5.	ATOM			ME'	r 396	18.125				49.39
	ATOM		-	GL		17.21				52.12
						16.64				
			22 CI	-						55.34
	ATOM		23 C						3 1.00	58.86
	MOTA	_	24 CI			_	5 3.44			63.28
_	ATOM			E1 GL						64.68
	MOTA			E1 GL						65.39
(50 ATOM	_							3 1.00	52.75
	ATOM	7	27 C	GL		, 17.5-				

5	ATOM	728	0	CT TT	205			•		
	MOTA	729	_	GLU HIS		17.071	,		1.00	53.96
	ATOM	730		HIS		18.851			1.00	50.25
	ATOM	731			· -	19.813			1.00	
	ATOM	732	_	HIS	_	20.271			1.00	
10		732		HIS		19.187	_ ·		1.00	
	ATOM	734			398	18.750		40.472	1.00	
	ATOM				398	18.374		38.608		
	ATOM	735			398	17.482		38.685		
	MOTA	736		-	398	17.688				55.81
15		737		HIS	398	20.999	3.084			47.44
13	MOTA	738		HIS	398	22.121	2.887			44.91
	MOTA	739		PRO	399	20.755				46.45
	ATOM	740	CD	PRO	399	19.443		42.721		
	ATOM	741	CA	PRO	399	21.785		42.586		47.27
20	MOTA	742	CB	PRO	399	21.127		43.793		45.35
20	ATOM	743	CG	PRO	399	19.660	5.561	43.504		47.40
	ATOM	744	C	PRO	399	23.086	4.270	42.958		47.72
	MOTA	745	0	PRO	399	23.078	3.233	43.627		44.70
	MOTA	746	N	\mathtt{GLY}	400	24.202	4.840	42.509		46.46
0.5	MOTA	747	CA	\mathtt{GLY}	400	25.506	4.281		1.00	41.57
25	MOTA	748	C	\mathtt{GLY}	400	25.907	3.047	42.813	1.00	39.84
	MOTA	749	0	\mathtt{GLY}	400	27.027	2.560	42.022	1.00	37.85
	MOTA	750	N	LYS	401	25.012	2.537	42.176	1.00	40.48
	ATOM	751	CA	LYS	401	25.315	1.344	41.180	1.00	36.39
	MOTA	752	CB	LYS	401	24.562		40.390	1.00	34.47
30	MOTA	. 753	CG	LYS	401	24.633	0.130	40.947	1.00	36.12
	ATOM	754	CD	LYS	401	24.288	-0.007	42.466	1.00	39.30
	MOTA	755	CE	LYS	401	24.459	-1.429	42.903	1.00	44.38
	ATOM	756	NZ	LYS	401	24.459	-1.605	44.408	1.00	46.68
	ATOM	757	C	LYS	401	24.969	-2.969	44.747	1.00	53.37
35	ATOM	758	0	LYS	401	24.141	1.485	38.911	1.00	32.34
	ATOM	759	N	LEU	402		2.308	38.531	1.00	31.16
	ATOM	760	CA	LEU	402	25.612	0.663	38.086	1.00	28.52
	MOTA	761	CB	LEU	402	25.358	0.658	36.648	1.00	29.06
	ATOM	762	CG	LEU	402	26.661	0.847	35.867	1.00	29.26
40	ATOM	763	CD1	LEU	402	27.278	2.242	36.029	1.00	24.67
	ATOM	764	CD2	LEU		28.623	2.310	35.310	1.00	27.47
	ATOM	765	C	LEU	402	26.312	3.277	35.482	1.00	24.93
	ATOM	766	0	LEU	402	24.755	-0.686	36.292	1.00	30.43
	ATOM	767	N	LEU	402	25.367	-1.727	36.535	1.00	31.36
45	ATOM	768	CA	LEU	403	23.552	-0.658	35.735	1.00	31.07
	ATOM	769	CB	LEU	403	22.873	-1.880	35.335	1.00	32.96
	ATOM	770	CG	LEU	403	21.361	-1.693	35.434	1.00	33.86
	ATOM	771	CD1		403	20.551	-2.991	35.415	1.00	39.29
	ATOM	772	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
50	ATOM	773	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
	ATOM	774		LEU	403	23.255	-2.218	33.899	1.00	30.06
	ATOM	775	0	LEU	403	22.543	-1.870	32.956	1.00	31.63
	MOTA	775 776	N	PHE	404	24.383	-2.893	33.733	1.00	29.19
	ATOM		CA	PHE	404	24.834	-3.256	32.403	1.00	28.93
55		777	CB	PHE	404	26.201	-3.929	32.493		30.05
22	ATOM	778	CG	PHE	404	27.305	-2.998	32.926		30.05
	ATOM	779	CD1	PHE	404	27.794	-3.033	34.228		30.78 32.91
	ATOM	780	CD2	PHE	404	27.848	-2.078	32.030		
	ATOM	781	CE1	PHE	404	28.816	-2.160	34.638		32.75
60	MOTA	782	CE2	PHE	404	28.864	-1.205	32.423		34.73
00	MOTA	783	CZ	PHE	404	29.350	-1.242	33.727		30.68
	ATOM	784	С	PHE	404	23.809	-4.181	31.756		31.43
						310	- · 	/56	1.00	30.80

			_		4.0.4	22 625	-4.175	30.538	1.00	28.09
5	ATOM	785	0	PHE	404	23.625	-4.175 -4.967	32.594		30.25
	ATOM	786	N	ALA	405	23.138		32.163	1.00	29.78
	MOTA	787	CA	ALA	405	22.104	-5.910	31.598	1.00	29.97
	ATOM	788	CB	ALA	405	22.745	-7.172	33.429	1.00	31.95
_	MOTA	789	C	ALA	405	21.309	-6.237	34.535	1.00	32.36
10	MOTA	790	0	ALA	405	21.785	-5.995	33.288	1.00	34.40
	MOTA	791	N	PRO	406	20.088	-6.779		1.00	35.81
	MOTA	792	CD	PRO	406	19.356	-7.102	32.053	1.00	36.41
	MOTA	793	CA	PRO	406	19.303	-7.101	34.490	1.00	35.38
	MOTA	794	CB	PRO	406	17.985	-7.654	33.935	1.00	36.49
15	MOTA	795	CG	PRO	406	17.922	-7.153	32.519	1.00	37.32
	ATOM	796	C	PRO	406	19.997	-8.084	35.433		38.34
	MOTA	797	0	PRO	406	19.698	-8.112	36.626	1.00	36.69
	MOTA	79E	N	ASN	407	20.924	-8.877	34.902	1.00	38.85
	MOTA	799	CA	ASN	407	21.652	-9.847	35.712	1.00	39.69
20	MOTA	800	CB	ASN	407	21.582	-11.243	35.083	1.00	44.10
	MOTA	801	CG	ASN	407	22.232	-11.306	33.711	1.00	37.78
	MOTA	802	OD1	ASN	407	22.345	-10.296	33.009	1.00	37.78 45.74
	MOTA	803	ND2	ASN	407	22.660	-12.503	33.319	1.00	38.12
	MOTA	804	C	ASN	407	23.100	-9.435	35.874		39.81
25	MOTA	805	0	ASN	407	23.965	-10.256	36.178	1.00	37.80
	MOTA	806	N	LEU	408	23.364	-8.149	35.671	1.00 1.00	36.89
	MOTA	807	CA	LEU	408	24.713	-7.631	35.799		36.09
	MOTA	808	CB	LEU	408	25.449	-7.720	34.459	1.00	35.09
	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	39.15
30	MOTA	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	36.85
	MOTA	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	40.55
	MOTA	812	С	LEU	408	24.670	-6.187	36.286	1.00	38.29
	MOTA	813	0	LEU	408	24.646	-5.248	35.491	1.00	39.50
	MOTA	814	N	LEU	409	24.644	-6.034	37.607 38.257	1.00	41.00
35	MOTA	815	CA	LEU	409	24.606	-4.733	39.184	1.00	43.69
	MOTA	816	CB	LEU	409	23.392	-4.658 -3.382	39.993	1.00	47.35
	MOTA	817	CG	LEU	409	23.164	-2.233	39.058	1.00	47.09
	MOTA	818	CD1	LEU	409	22.848		40.976	1.00	49.38
	MOTA	819	CD2	LEU	409	22.014 25.894		39.060	1.00	41.80
40	MOTA	820	С	LEU	409	25.694	-5.358	39.960	1.00	41.00
	MOTA	821	0	LEU	409	_		38.727		39.23
	MOTA	822	N	LEU	410 410	26.676 27.931		39.423		40.45
	ATOM	823	CA CB	LEU LEU	410	29.106		38.442		41.59
15	MOTA	824 825	CG	LEU	410	29.457		37.716		44.87
45	MOTA	826	CD1	LEU	410	30.972		37.554		
	MOTA	827	CD1	LEU		28.949		38.484		
	MOTA	828	CD2	LEU		27.946		40.132		
	MOTA	829		LEU		27.361				
50	ATOM	830		ASP		28.610				
50		831		ASP		28.717				
	MOTA	832		ASP		28.490				
	MOTA	833		ASP		29.655				
	ATOM					29.537				
55	ATOM	834				30.680				
55		835		ASP		30.088				
	MOTA	836		ASP ASP		30.030				
	MOTA	837		ASP		30.295				
	MOTA	838		ARG		31.554				
<i>c</i> 0	MOTA	839		ARG		31.60				
60		840		ARG		30.97				
	MOTA	841		טאה		30.57.				

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5	MOTA	842	CD	ARG	412	31.644	5.580	43.219	1.00	54.61
	MOTA	843	NE	ARG	412	33.071	5.615	42.912	1.00	56.53
	MOTA	844	CZ	ARG	412	33.827	6.708	42.985	1.00	61.90
	MOTA	845	NH1	ARG	412	33.291	7.866	43.356	1.00	63.48
	MOTA	846	NH2	ARG	412	35.120	6.645	42.682	1.00	61.21
10	MOTA	847	С	ARG	412	32.771	1.026	42.429	1.00	50.29
	ATOM	848	Ō	ARG	412	33.628	0.866	41.561	1.00	51.02
	ATOM	849	И	ASN	413	32.844				
	ATOM	850	CA	ASN	413		0.469	43.633	1.00	51.94
	ATOM	851	CB			33.969	-0.375	44.021	1.00	53.15
15				ASN	413	33.719	-0.980	45.403	1.00	55.88
13	ATOM	852	CG	ASN	413	33.654	0.073	46.496	1.00	57.99
	ATOM	853	OD1	ASN	413	33.697	1.276	46.223	1.00	58.27
	ATOM	854	NDS	ASN	413	33.551	-0.375	47.742	1.00	57.90
	ATOM	855	C	ASN	413	34.235	-1.480	43.013	1.00	53.95
20	ATOM	856	0	ASN	413	35.386	-1.743	42.659	1.00	53.67
20	MOTA	857	N	GLN	414	33.173	-2.129	42.547	1.00	55.33
	ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.42
	MOTA	859	CB	GLN	414	31.991	-3.904	41.343	1.00	55.44
	MOTA	860	CG	${ t GLN}$	414	31.645	-4.933	42.391	1.00	56.07
	MOTA	861	CD	GLN	414	30.203	-5.376	42.336	1.00	57.40
25	MOTA	862	OE1	GLN	414	29.296	-4.536	42.402	1.00	60.22
	MOTA	863	NE2	${ t GLN}$	414	29.973	-6.664	42.199	1.00	57.27
	MOTA	864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
	MOTA	865	0	GLN	414	34.654	-3.265	39.578	1.00	56.16
	MOTA	866	N	\mathtt{GLY}	415	33.398	-1.430	39.910	1.00	57.07
30	MOTA	867	CA	\mathtt{GLY}	415	33.849	-0.806	38.680	1.00	58.51
	MOTA	868	C	\mathtt{GLY}	415	35.350	-0.582	38.689	1.00	61.10
	MOTA	869	0	\mathtt{GLY}	415	36.023	-0.748	37.671	1.00	59.47
	ATOM	870	N	LYS	416	35.877	-0.211	39:851	1.00	62. 7 7
	MOTA	871	CA	LYS	416	37.305	0.041	40.011	1.00	65.49
35	MOTA	872	CB	LYS	416	37.634	0.262	41.491	1.00	66.04
	MOTA	873	CG	LYS	416	38.121	1.663	41.823	1.00	68.71
	MOTA	874	CD	LYS	416	37.078	2.439	42.613	1.00	70.98
	MOTA	875	CE	LYS	416	37.404	2.448	44.100	1.00	71.84
	MOTA	876	NZ	LYS	416	36.225	2.079	44.933	1.00	71.95
40	MOTA	877	C	LYS	416	38.159	-1.105	39.472	1.00	66.41
	MOTA	878	0	LYS	416	39.361	-0.946	39.269	1.00	67.15
	MOTA	879	N	CYS	417	37.538	-2.257	39.238	1.00	67.33
	MOTA	880	CA	CYS	417	38.270	-3.414	38.741	1.00	68.16
	ATOM	881	CB	CYS	417	37.951	-4.642		1.00	70.88
45	MOTA	882	SG	CYS	417	38.592	-4.549	41.301	1.00	76.09
	MOTA	883	С	CYS	417	38.015	-3.736	37.270	1.00	67.54
	ATOM	884	0	CYS	417	38.632	-4.653	36.720	1.00	68.48
	MOTA	885	N	VAL	418	37.111	-2.994	36.631	1.00	64.67
	MOTA	886	CA	VAL	418	36.817	-3.226	35.218	1.00	59.97
50	MOTA	887	CB	LAV	418	35.326	-2.917	34.879	1.00	59.60
	MOTA	888	CG1	VAL	418	34.971	-1.503	35.284	1.00	59.13
	ATOM	889	CG2	VAL	418	35.072	-3.121	33.391	1.00	54.85
	ATOM	890	C	VAL	418	37.739	-2.362	34.355	1.00	58.37
	ATOM	891	Ō	VAL	418	37.799	-1.140	34.512	1.00	55.44
55	ATOM	892	N	GLU	419	38.463	-3.012	33.450	1.00	56.02
	ATOM	893	CA	GLU	419	39.403	-2.328	32.570	1.00	
	ATOM	894	CB	GLU	419	40.149	-3.351	31.710	1.00	54.28 57.57
	ATOM	895	CG	GLU	419	39.385	-3.331	30.468	1.00	
	ATOM	896	CD	GLU	419	40.179	-3.779 -4.722	29.584	1.00	60.87
60	ATOM	897	OE1	GLU	419	40.432	-5.870	30.011	1.00	63.34
	ATOM	898	OE1	GLU	419	40.432	-4.313	28.462		64.90
	0		252	210	-117	40.540	-4.213	40.402	1.00	63.18

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5	MOTA	899	С	GLU	419	38.761	-1.281	31.662		52.05
•	ATOM	900	0	GLU	419	37.665	-1.481	31.131		49.82
	ATOM	901	N	GLY	420	39.465	-0.165	31.491		49.45
	MOTA	902	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
	MOTA	903	C	GLY	420	37.895	1.767	31.254	1.00	44.55
10	ATOM	904	0	GLY	420	37.417	2.705	30.619	1.00	42.08
	MOTA	905	N	MET	421	37.503	1.471	32.488	1.00	43.41
	MOTA	906	CA	MET	421	36.449	2.248	33.123	1.00	42.48
	MOTA	907	CB	MET	421	35.306	1.327	33.554	1.00	42.34
	MOTA	908	CG	MET	421	34.590	0.635	32.396	1.00	38.22
15	MOTA	909	SD	MET	421	32.927	0.102	32.843	1.00	38.56
	MOTA	910	CE	MET	421	32.003	1.699	32.766	1.00	35.54
	ATOM	911	C	MET	421	36.923	3.059	34.312	1.00	41.64
	MOTA	912	0	MET	421	36.113	3.512	35.111	1.00	39.77
	MOTA	913	N	\mathtt{VAL}	422	38.232	3.256	34.430	1.00	43.42
20	MOTA	914	CA	$_{ m LAV}$	422	38.757	4.019	35.557	1.00	44.79
	MOTA	915	CB	VAL	422	40.285	4.248	35.433	1.00	46.54 48.25
	MOTA	916	CG1	LAV	422	40.595	5.086	34.206	1.00	46.24
	MOTA	917	CG2	VAL	422	40.813	4.920	36.696	1.00	44.09
	MOTA	918	С	JAV	422	38.056	5.372	35.689	1.00	44.12
25	ATOM	919	0	VAL	422	37.691	5.783	36.783 34.570	1.00	42.07
	MOTA	920	N	GLU	423	37.846	6.055	34.570	1.00	40.24
	MOTA	921	CA	GLU	423	37.192	7.356 8.338	33.684	1.00	44.02
	MOTA	922	CB	GLU	423	37.909	8.467	33.893	1.00	50.04
	MOTA	923	CG	GLU	423	39.411 40.096	9.158	32.719	1.00	55.64
30	MOTA	924	CD	GLU	423	39.539	10.156	32.205	1.00	56.66
	ATOM	925	OE1	GLU	423 423	41.188	8.703	32.306	1.00	58.02
	MOTA	926	OE2 C	GLU GLU	423	35.704	7.337	34.250	1.00	35.77
	ATOM	927	0	GLU	423	34.881	7.955	34.919	1.00	33.20
35	MOTA	928 929	И	ILE	424	35.345	6.617	33.197	1.00	36.16
33	MOTA MOTA	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
	MOTA	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
	MOTA	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
	MOTA	933	CG1	ILE	424	34.204	4.617	31.296	1.00	34.46
40	MOTA	934	CD1	ILE	424	33.857	3.955	29.978	1.00	34.67
10	ATOM	935	C	ILE	424	32.890	6.035	33.685	1.00	28.89
	ATOM	936	0	ILE	424	31.729	6.443	33.632	1.00	
	MOTA	937		PHE	425	33.261	5.091	34.542	1.00	29.26
	ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	
45	MOTA	939	CB	PHE	425	32.903	3.529	36.423		
	MOTA	940	CG	PHE	425	31.948				
	MOTA	941	CD1	PHE	425	31.124				
	MOTA	942	CD2	PHE	425	31.881				
	ATOM	943	CE1	PHE	425	30.244				
50	ATOM	944	CE2	PHE	425	31.010				
	MOTA	945	CZ	PHE	425	30.189				
	ATOM	946	C	PHE	425	31.594				
	ATOM	947	0	PHE	425	30.368				
	ATOM	948		ASP		32.415				
55	MOTA	949	CA	ASP		31.893				
	ATOM	950		ASP		33.031				
	ATOM	951		ASP		33.455				
	ATOM	952				32.767				
	ATOM	953				34.480				
60		954		ASP		31.133				
	MOTA	955	5 0	ASP	426	30.154	9.175	37.25	7 1.00	31.34

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5	ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
	ATOM	957	CA	MET	427	30.919	9.736	34.675	1.00	28.63
	MOTA	958	CB	MET	427	31.744	9.912	33.407	1.00	26.83
	ATOM	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
10	MOTA	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
10	MOTA	961	CE	MET	427	35.409	11.753	32.643	1.00	44.60
	MOTA	962	С	MET	427	29.526	9.202	34.324	1.00	28.70
	ATOM	963	0	MET	427	28.536	9.947	34.302	1.00	25.01
	MOTA	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	ATOM	965	CA	LEU	428	28.173	7.292	33.730	1.00	27.60
15	MOTA	966	CB	LEU	428	28.379	5.824	33.332	1.00	28.00
	ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
	ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	MOTA	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	ATOM	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
20	MOTA	971	0	LEU	428	26.041	7.743	34.743	1.00	27.07
	MOTA	972	N	LEU	429	27.701	7.147	36.126	1.00	30.40
	MOTA	973	CA	LEU	429	26.859	7.251	37.323 ·	1.00	30.59
	MOTA	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
	ATOM	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
25	MOTA	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
	MOTA	977	CD2	LEU	429	26.825	4.573	38.903	1.00	34.66
	MOTA	978	С	LEU	429	26.319	8.681	37.466	1.00	30.46
	MOTA	979	0	LEU	429	25.143	8.901	37.769	1.00	28.40
	ATOM	980	N	ALA	430	27.193	9.656	37.237	1.00	31.34
30	MOTA	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
	ATOM	982	CB	ALA	430	28.017	11.951	37.078	1.00	31.29
	MOTA	983	С	ALA	430	25.696	11.387	36.344	1.00	31.04
	MOTA	984	0	ALA	430	24.753	12.107	36.674	1.00	30.79
25	MOTA	985	Ŋ	THR	431	25.802	10.854	35.128	1.00	30.30
35	MOTA	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
	MOTA	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	MOTA	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
40	ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
40	MOTA	991	0	THR	431	22.402	11.099	34.397	1.00	26.18
	MOTA	992	N	SER	432	23.520	9.253	35.037	1.00	28.11
	ATOM . ATOM	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
	ATOM	994 995	CB OG	SER SER	432 432	22.639	7.177	36.008	1.00	33.11
45	ATOM	996	C	SER	432	21.454 21.651	6.412	36.136	1.00	36.92
73	MOTA	997	0	SER	432	20.433	9.399 9.576	36.589	1.00	31.49
	ATOM	998	N	ASER		20.433	9.901	36.613 37.496	0.75	30.09
	ATOM	999	N	BSER		22.474	9.901	37.500	0.75	32.09
	ATOM	1000	CA	ASER		22.002	10.715	38.605	0.25	31.10
50	ATOM	1000	CA	BSER		21.985	10.715		0.75	35.68
50	ATOM	1001	CB	ASER		23.185	11.097	38.608 39.502	0.25	32.21 37.18
	ATOM	1002	CB	BSER		23.145	11.104	39.502	0.75	31.45
	MOTA	1003		ASER		22.823	12.090	40.443	0.25	44.09
	ATOM	1004		BSER		23.785	9.953	40.443	0.75	
55	ATOM	1005		ASER		23.765	11.971	38.091	0.25	29.52 35.01
55	ATOM	1007		BSER		21.295	11.971	38.091	0.75	32.88
	ATOM	1007		ASER		20.257	12.373	38.612	0.25	
	ATOM	1009		BSER		20.257	12.373	38.622	0.75	35.34
	ATOM	1010		ARG	434	20.264	12.579	37.054	1.00	33.42
60	ATOM	1011		ARG	434	21.867	13.788	36.470	1.00	33.38 34.19
30	ATOM	1011		ARG	434	22.239	14.354	35.400	1.00	33.89
	111 011	-0-2	-1	23160	174	22.23	74.774	22.400	1.00	رن. در

5	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
	ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
	ATOM	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
	ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
	MOTA	1017	NH1	ARG	434	20.132	19.049	36.428	1.00	40.70
10	MOTA	1018	NH2	ARG	434	20.175	19.998	34.337	1.00	38.78
	ATOM	1019	С	ARG	434	19.937	13.491	35.873	1.00	33.48
	MOTA	1020	0	ARG	434	18.996	14.266	36.053	1.00	30.54
	ATOM	1021	N	PHE	435	19.831	12.371	35.158	1.00	34.68
	ATOM	1022	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
15	ATOM	1023	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
	ATOM	1024	CG	PHE	435	19.240	10.779	32.386	1.00	37.63
	ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
	ATOM	1026	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
	MOTA	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
20	ATOM	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
20	MOTA	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
	ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49
	ATOM	1031	Ö	PHE	435	16.361	12.135	35.496	1.00	34.78
	ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
25	ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
23	ATOM	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
	ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	ATOM	1036	CD	ARG	436	17.648	8.459	40.810	1.00	48.09
	ATOM	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
30	ATOM	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
50	MOTA	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
	MOTA	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	ATOM	1041		ARG	436	16.576	12.302	38.493	1.00	40.40
	ATOM	1042		ARG	436	15.382	12.458	38.730	1.00	41.49
35	MOTA	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02
33	MOTA	1044		MET	437	17.090	14.546	39.245	1.00	41.02
	ATOM	1045		MET	437	18.329	15.427	39.440	1.00	40.29
	ATOM	1046		MET	437	16.099	15.221	38.299	1.00	40.81
	ATOM	1047		MET	437	15.111	15.805	38.734	1.00	42.46
40	MOTA	1048		MET	438	16.367	15.127	37.001	1.00	39.02
	ATOM	1049		MET	438	15.510	15.732	35.988	1.00	40.11
	ATOM	1050		MET	438	16.237	15.793	34.651	1.00	38.16
	ATOM	1051		MET	438	17.352	16.794	34.601	1.00	41.52
	ATOM	1052		MET	438	17.999	16.862	32.943	1.00	43.94
45	MOTA	1053		MET	438	16.698	17.748	32.096	1.00	39.96
, ,	MOTA	1054		MET	438	14.221	14.964	35.783	1.00	37.72
	MOTA	1055		MET	438	13.305	15.451	35.125	1.00	36.82
	MOTA	1056		ASN	439	14.155	13.759	36.337	1.00	38.81
	ATOM	1057		ASN	439	12.981	12.919	36.174	1.00	40.77
50	ATOM	1058		ASN	439	11.762	13.556	36.847	1.00	44.52
50	ATOM	1059		ASN	439	10.566	12.620	36.887	1.00	48.29
	MOTA	1060		ASN	439	10.721	11.400	36.964	1.00	48.48
	ATOM	1061		ASN	439	9.365	13.189	36.829	1.00	50.23
	ATOM	1062		ASN	439	12.725	12.744	34.677	1.00	39.36
55	MOTA	1062		ASN	439	11.637	13.037	34.172	1.00	37.76
رر	MOTA	1064		LEU	440	13.749	12.274	33.972	1.00	37.75
	ATOM	1065		LEU	440	13.749	12.052	32.532	1.00	35.22
	ATOM	1066		LEU	440	14.999	11.576	31.987	1.00	34.70
	ATOM	1067		LEU	440	15.022	11.467	30.462	1.00	35.45
60	ATOM	1067		LEU	440	14.890	12.862	29.869	1.00	35.43
50	ATOM	1069		LEU	440	16.297	10.795	29.889	1.00	35.30
	HI OM	£003	112	ں ندید	770	10.231	20.193	27.77	2.00	JJ.JU

5	ATOM	1070	С	LEU	440	12.587	11.024	32.196	1:00	36.48
	MOTA	1071	0	LEU	440	12.518	9.967	32.826	1.00	37.36
	ATOM	1072	N	${ t GLN}$	441	11.763	11.328	31.197	1.00	36.82
	MOTA	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
	ATOM	1074	CB	${ t GLN}$	441	9.431	11.211	30.443	1.00	38.23
10	MOTA	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	MOTA	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
	ATOM	1078	NE2	GLN	441	9`.119	11.132	33.818	1.00	44.06
	MOTA	1079	С	GLN	441	11.099	9.565	29.585	1.00	38.48
15	ATOM	1080	0	GLN	441	11.923	9.976	28.763	1.00	35.80
	MOTA	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
	MOTA	1082	CA	\mathtt{GLY}	442	10.792	7.468	28.401	1.00	37.72
	MOTA	1083	С	GLY	442	10.599	8.112	27.043	1.00	36.88
	MOTA	1084	0	GLY	442	11.381	7.877	26.123	1.00	33.72
20	ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	MOTA	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
	MOTA	1087	CB	GLU	443	7.956	10.379	25.764	1.00	41.57
	MOTA	1088	CG	GLU	443	6.723	9.488	25.879	1.00	47.76
	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
25	MOTA	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
	MOTA	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13
	MOTA	1092	С	GLU	443	10.408	10.551	25.311	1.00	35.27
	MOTA	1093	0	GLU	443	10.759	10.704	24.145	1.00	33.85
	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	.32.09
30	MOTA	1095	CA	GLU	444	12.097	12.095	26.126	1.00	33.92
	MOTA	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
	MOTA	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
	MOTA	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	MOTA	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
35	MOTA	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
	MOTA	1101	С	GLU	444	13.356	11.305	25.770	1.00	33.59
	MOTA	1102	0	GLU	444	14.085	11.670	24.842	1.00	33.35
	ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
4.0	MOTA	1104		PHE	445	14.753	9.357	26.276	1.00	32.49
40	MOTA	1105		PHE	445	14.703	8.139	27.203	1.00	29.35
	MOTA	1106		PHE	445	15.667	7.047	26.828	1.00	30.78
	MOTA	1107		PHE	445	17.036	7.201	27.030		
	ATOM	1108		PHE	445	15.205	5.863	26.266	1.00	30.62
15	ATOM	1109		PHE	445	17.933	6.195	26.675	1.00	28.67
45	ATOM	1110		PHE	445	16.095	4.848	25.908	1.00	31.37
	ATOM	1111		PHE	445	17.460	5.015	26.113	1.00	30.37
	ATOM	1112		PHE	445	14.850	8.885	24.829	1.00	31.11
	MOTA	1113		PHE	445	15.924	8.947	24.221 24.266	1.00	32.20
50	ATOM ATOM	1114 1115		VAL VAL	446 446	13.739 13.787	8.415 7.943	24.266	1.00	28.63 27.94
50	ATOM	1115		VAL	446	12.478	7.193	22.478	1.00	28.48
	ATOM	1117		VAL	446	12.318	5.939	23.343	1.00	29.61
	ATOM	1118		VAL	446	11.265	8.092	22.607	1.00	27.23
	ATOM	1119		VAL	446	14.099	9.064	21.900	1.00	27.23
55	ATOM	1119		VAL	446	14.781	8.837	20.904	1.00	28.07
,,	ATOM	1120		CYS	447	13.619	10.275	20.904	1.00	28.07
	ATOM	1121		CYS	447	13.019	11.394	21.272	1.00	29.14
	ATOM	1122		CYS	447	13.156	12.653	21.272	1.00	28.90
	ATOM	1123		CYS	447	11.389	12.591	21.309	1.00	35.68
60	ATOM	1125		CYS	447	15.420	11.677	21.328	1.00	28.03
00	ATOM	1126		CYS	447	16.063	11.885	20.302	1.00	29.34
			_							

5	ATOM	1127	N	LEU	448	15.969	11.686	22.538		27.28
	MOTA	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	MOTA	1129	CB	LEU	448	17.733	11.932	24.220	1.00	27.72
	MOTA	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
	MOTA	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
10	MOTA	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
	ATOM	1133	C	LEU	448	18.245	10.902	22.008	1.00	27.62
	MOTA	1134	0	LEU	448	19.207	11.252	21.327	1.00	25.10
	MOTA	1135	N	LYS	449'	17.905	9.621	22.162	1.00	25.16
	MOTA	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55 28.99
15	ATOM	1137	CB	LYS	449	18.135	7.185	21.900 21.694	1.00 1.00	34.70
	MOTA	1138	CG	LYS	449	19.134	6.052		1.00	32.67
	MOTA	1139	CD	LYS	449	18.737	4.789	22.459 22.220	1.00	31.87
	MOTA	1140	CE	LYS	449	17.267	4.419	22.220	1.00	29.14
	MOTA	1141	ΝZ	LYS	449	17.022	2.967	19.990	1.00	25.88
20	MOTA	1142	C	LYS	449	18.626	8.749 8.489	19.296	1.00	25.93
	MOTA	1143	0	LYS	449	19.610 17.482	9.197	19.480	1.00	26.07
	MOTA	1144	N	SER	450 450	17.323	9.421	18.052	1.00	27.24
	MOTA	1145	CA	SER SER	450	15.857	9.705	17.721	1.00	32.24
25	ATOM	1146	CB OG	SER	450	15.098	8.519	17.779	1.00	34.94
25	MOTA	1147 1148		SER	450	18.176	10.607	17.618	1.00	26.78
	ATOM	1148		SER	450	18.763	10.598	16.535	1.00	25.85
	ATOM ATOM	1150		ILE	451	18.231	11.632	18.463	1.00	26.94
	ATOM	1151		ILE	451	19.032	12.810	18.155	1.00	26.13
30	MOTA	1152		ILE	451	18.950	13.850	19.291	1.00	27.72
50	MOTA	1153		ILE	451	20.019	14.929	19.101	1.00	20.53
	ATOM	1154		ILE	451	17.553	14.475	19.322	1.00	29.49
	ATOM	1155		ILE	451	17.377	15.473	20.447	1.00	36.24
	ATOM	1156		ILE	451	20.489	12.381	17.989	1.00	24.88
35	ATOM	1157		ILE	451	21.161	12.771	17.034	1.00	26.96
	ATOM	1158	3 N	ILE	452	20.977	11.582	18.931	1.00	22.72
	ATOM	1159	CA	ILE	452	22.359	11.120	18.880	1.00	21.95
	MOTA	1160) CB	ILE	452	22.660	10.155	20.050	1.00	23.57
	MOTA	1161	L CG2	ILE	452	23.982	9.435	19.804	1.00	22.10
40	MOTA	1162	2 CG1	ILE	452	22.718	10.949	21.371	1.00	21.70
	MOTA	1163		ILE	452	22.768	10.060	22.624	1.00	25.30
	MOTA	1164		ILE	452	22.656		17.557		
	. ATOM	116		ILE	452	23.650		16.885		
	MOTA	116		LEU	453	21.779		17.173		
45	MOTA	116'		LEU	453	21.984		15.935 15.733		
	MOTA	116		LEU	453	20.843				
	ATOM	116		LEU		20.712 21.815				
	ATOM	117				19.328				
50	ATOM	117				22.092				
50		117		LEU LEU		22.962				
	ATOM	117		LEU		21.220				
	MOTA	117		LEU		21.220				
	MOTA	117		LEU		19.852				
55	MOTA ATOM	117 117		LEU		18.737				
33		117				17.405				
	MOTA MOTA	117				19.037				
	MOTA	117		LEU		22.292				
	MOTA	118		LEU		22.778				
60		118		ASN		22.638				
00	MOTA	118		ASN		23.604				26.79
	0.7									

5	MOTA	1184	CB	ASN	455	23.284	14.998	16.224		26.20
	ATOM	1185	CG	ASN	455	24.174	16.217	16.419	1.00	27.26
	MOTA	1186	OD1	ASN	455	24.171	17.134	15.602	1.00	30.83
	ATOM	1187	MD3	ASN	455	24.931	16.230	17.506	1.00	27.16
	MOTA	1188	С	ASN	455	25.062	13.782	14.954	1.00	30.63
10	MOTA	1189	0	ASN	455	25.965	14.517	14.525	1.00	27.69
	MOTA	1190	N	SER	456	25.268	12.569	15.461	1.00 .	30.48
	ATOM	1191	CA	SER	456	26.572	11.928	15.579	1.00	35.26
	MOTA	1192	CB	SER	456	26.393	10.393	15.505	1.00	39.69
	MOTA	1193	OG	SER	456	25.871	9.953	14.243	1.00	30.73
15	MOTA	1194	C	SER	456	27.627	12.344	14.562	1.00	35.56
	MOTA	1195	0	SER	456	28.599	13.041	14.884	1.00	33.00
	ATOM	1196	N	GLY	457	27.437	11.886	13.334	1.00	33.88
	MOTA	1197	CA	\mathtt{GLY}	457	28.393	12.189	12.292	1.00	36.77
	MOTA	1198	С	GLY	457	27.876	13.017	11.136	1.00	37.02
20	MOTA	1199	0	\mathtt{GLY}	457	28.310	12.805	10.013	1.00	38.66
	MOTA	1200	N	VAL	458	26.967	13.956	11.392	1.00	39.12
	MOTA	1201	CA	VAL	458	26.438	14.802	10.317	1.00	43.81
	ATOM	1202	CB	VAL	458	25.231	15.648	10.755	1.00	44.25
	MOTA	1203	CG1	VAL	458	24.209	15.713	9.631	1.00	44.51
25	MOTA	1204	CG2	VAL	458	24.638	15.098	12.013	1.00	50.53
	MOTA	1205	С	VAL	458	27.472	15.801	9.817	1.00	46.72
	MOTA	1206	0	VAL	458	27.391	16.265	8.681	1.00	47.08
	MOTA	1207		TYR	459	28.432	16.144	10.670	1.00	50.74
	MOTA	1208		TYR	459	29.456	17.114	10.301	1.00	55.43 56.62
30	MOTA	1209		TYR	459	29.647	18.129	11.433	1.00	59.34
	MOTA	1210		TYR	459	28.375	18.870	11.781	1.00	60.73
	ATOM	1211		TYR	459	28.094	19.229	13.095	1.00	62.14
	MOTA	1212		TYR	459	26.900	19.867	13.429 10.795	1.00	62.14
	MOTA	1213		TYR	459	27.430	19.175	10.795	1.00	63.83
35	MOTA	1214		TYR	459	26.234	19.812 20.154	12.437	1.00	62.88
	MOTA	1215		TYR	459	25.976	20.154	12.437	1.00	62.56
	MOTA	1216		TYR	459	24.790	16.489	9.928	1.00	57.21
	ATOM	1217		TYR	459 459	30.791 31.793	17.189	9.798	1.00	56.86
40	MOTA	1218		TYR	459	30.800	15.173	9.750	1.00	59.22
40	ATOM	1219 1220		THR THR	460	32.018	14.474	9.366	1.00	62.25
	MOTA			THR	460	32.502	13.531	10.499	1.00	63.07
	MOTA	1221		THR	460	33.474		9.983		67.80
	ATOM	1223	2 OG1 3 CG2	THR	460	31.344		11.084		60.23
45	ATOM ATOM	1223		THR	460	31.759		8.086		63.54
43	ATOM	1225		THR	460	32.457	12.708	7.782		
	ATOM	1226		PHE	461	30.758	14.113	7.326		
	ATOM	122		PHE	461	30.395		6.080		
	ATOM	1228		PHE	461	29.052	13.975	5.563		
50	MOTA	122		PHE	461	27.867				66.30
50	MOTA	123		PHE	461	26.657				
	MOTA	123			461	27.963		6.085		
	MOTA	123			461	25.562				
	ATOM	123			461	26.872				
55	MOTA	123		PHE	461	25.670				
,,	ATOM	123		PHE	461	31.463				
	MOTA	123		PHE	461	32.181				
	ATOM		7 N	LEU		31.542				
	ATOM	123		LEU		32.511				
60	ATOM '		9 CB	LEU		32.080				
00	MOTA		0 C	LEU		32.810				
	ATOM	I O I	_			/				

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5	ATOM	1241	0	LEU	462	33.725	14.590	2.680	1.00	73.45
	ATOM	1242	N	SER	463	32.043	14.141	1.253	1.00	73.22
	ATOM	1243	CA	SER	463	32.262	15.343	0.449	1.00	72.61
	MOTA	1244	CB	SER	463	32.544	14.942	-1.005	1.00	73.38
	ATOM	1245	C	SER	463	31.126	16.362	0.491	1.00	71.17
10	MOTA	1246	0	SER	463	30.455	16.528	1.511	1.00	72.05
	MOTA	1247	N	SER	464	30.932	17.049	-0.633	1.00	68.86
	MOTA	1248	CA	SER	464	29.892	18.063	-0.759	1.00	66.06
	ATOM	1249	CB	SER	464	30.514	19.457	-0.704	1.00	66.26
	MOTA	1250	C	SER	464	29.108	17.887	-2.060	1.00	63.72
15	ATOM	1251	Ō	SER	464	28.657	18.862	-2.662	1.00	62.88
	MOTA	1252	N	THR	465	28.954	16.638	-2.493	1.00	60.93
	ATOM	1253	CA	THR	465	28.205	16.343	-3.709	1.00	57.47
	MOTA	1254	CB	THR	465	28.185	14.824	-4.004	1.00	57.80
	MOTA	1255	OG1	THR	465	27.525	14.135	-2.934	1.00	54.75
20	MOTA	1256	CG2	THR	465	29.606	14.287	-4.149	1.00	57.49
20			CGZ		465			-3.523		54.93
	MOTA	1257		THR		26.767	16.824		1.00	
	MOTA	1258	0	THR	465	26.349	17.129	-2.407	1.00	54.26
	MOTA	1259	N	LEU	466	26.013	16.892	-4.614	1.00	51.85
25	MOTA	1260	CA	LEU	466	24.625	17.330	-4.550	1.00	49.25
25	MOTA	1261	CB	LEU	466	24.013	17.349	-5.956	1.00	48.74
	ATOM	1262	CG	LEU	466	22.953	18.415	-6.253	1.00	48.72
	ATOM	1263	CD1	LEU	466	22.156	18.002	-7.482	1.00	48.32
	ATOM	1264	CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
30	MOTA	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
30	MOTA	1266	O N	LEU	466	22.961	16.845	-2.883	1.00	45.90
	ATOM	1267 1268	N C7	LYS LYS	467	24.093	15.099	-3.750	1.00	46.47
	ATOM	1269	CA	LYS	467 467	23.399 23.802	14.100 12.693	-2.947	1.00	47.45
	ATOM ATOM	1270	CB CG	LYS	467	22.829	11.602	-3.395 -2.974	1.00	49.38 52.70
35	MOTA	1271	CD	LYS	467	23.561	10.301	-2.682	1.00	56.48
55	ATOM	1271	CE	LYS	467	23.105	9.180	-3.604	1.00	59.54
	ATOM	1273	NZ	LYS	467	24.150	8.117	-3.732	1.00	61.22
	ATOM	1274	C	LYS	467	23.738	14.284	-1.472	1.00	46.89
	ATOM	1275	0	LYS	467	22.884	14.108	-0.604	1.00	46.06
40	ATOM	1276	И	SER	468	24.989	14.644	-1.202	1.00	45.82
-10	ATOM	1277	CA	SER	468	25.457	14.854	0.160	1.00	46.82
	MOTA	1278	CB	SER	468	26.976	15.050	0.173	1.00	47.85
	MOTA	1279		SER	468	27.407	15.537	1.435	1.00	55.73
	ATOM	1280		SER	468	24.778	16.063	0.790	1.00	44.24
45	ATOM	1281		SER	468	24.473	16.062	1.983	1.00	42.98
7.5	ATOM	1282		LEU	469	24.547	17.100	-0.011	1.00	42.33
	ATOM	1283		LEU	469	23.890	18.301	0.486	1.00	40.42
	ATOM	1284		LEU	469	24.002	19.427	-0.545	1.00	44.47
	ATOM	1285		LEU	469	25.438	19.874	-0.849	1.00	46.70
50	ATOM	1286		LEU	469	25.514	20.477	-2.246	1.00	46.70
50	ATOM	1287		LEU	469	25.890	20.477	0.199	1.00	47.32
	ATOM	1288		LEU	469	22.423	17.996	0.786	1.00	39.06
	ATOM	1289		LEU	469	21.856	18.505	1.760	1.00	34.97
	ATOM	1289		GLU	470	21.836	17.151	-0.046	1.00	35.46
55	ATOM	1291		GLU	470	20.418	16.768	0.145	1.00	34.38
22	ATOM	1291		GLU	470	19.914	15.768	-1.052	1.00	38.02
	ATOM	1292		GLU	470	19.772	16.773	-2.329	1.00	42.67
	ATOM	1293		GLU	470	19.772	15.773	-3.509	1.00	48.30
	ATOM	1294		GLU	470	19.339	13.923	-3.538	1.00	50.53
60	ATOM	1295		GLU	470	19.671	16.463	-4.412	1.00	51.06
00	ATOM	1297		GLU	470		15.916	1.403	1.00	34.37
	AIOM	1431	_	GLU	± / U	20.290	13.310	1.403	1.00	34.3/

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5	ATOM	1298	0	GLU	470	19.321	16.035	2.157	1.00	32.60
	MOTA	1299	N	GLU	471	21.274	15.046	1.606	1.00	34.66
	ATOM	1300	CA	GLU	471	21.309	14.162	2.766	1.00	35.68
	MOTA	1301	CB	GLU	471	22.515	13.222	2.671	1.00	34.57
	MOTA	1302	CG	GLU	471	22.376	12.122	1.614	1.00	37.98
10	MOTA	1303	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
	MOTA	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12 32.11
	MOTA	1305	OE2	GLU	471	21.974	10.061	2.737 4.052	1.00	34.79
	MOTA	1306	C	GLU	471	21.393	14.983	4.052	1.00	32.80
1.5	MOTA	1307	0	GLU	471	20.596	14.793 15.898	4.112	1.00	33.93
15	ATOM	1308	N	LYS	472	22.358 22.518	16.739	5.291	1.00	35.58
	MOTA	1309	CA	LYS	472 472	23.683	17.710	5.097	1.00	39.11
	MOTA	1310	CB	LYS	472 472	25.050	17.710	5.138	1.00	41.47
	ATOM	1311	CG	LYS LYS	472	26.080	17.957	5.794	1.00	46.97
20	MOTA	1312	CD CE	LYS	472	27.445	17.286	5.862	1.00	48.40
20	ATOM	1313	NZ	LYS	472	27.445	16.702	4.547	1.00	51.55
	MOTA	1314 1315	C	LYS	472	21.237	17.523	5.582	1.00	34.78
	MOTA MOTA	1316	0	LYS	472	20.795	17.607	6.724	1.00	33.95
	ATOM	1317	И	ASP	473	20.643	18.097	4.545	1.00	33.47
25	ATOM	1317	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
23	ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
	MOTA	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24
	MOTA	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
	ATOM	1322		ASP	473	17.750	21.396	3.932	1.00	45.59
30	MOTA	1323		ASP	473	18.339	17.998	5.338	1.00	32.93
50	MOTA	1324		ASP	473	17.642	18.416	6.264	1.00	32.87
	ATOM	1325		HIS	474	18.199	16.784	4.827	1.00	32.74
	MOTA	1326		HIS	474	17.185	15.882	5.343	1.00	32.21
	MOTA	1327		HIS	474	17.185	14.575	4.568	1.00	32.79
35	ATOM	1328	CG	HIS	474	16.047	13.675	4.924	1.00	36.22
	MOTA	1329	· CD2	HIS	474	14.711	13.813	4.750	1.00	38.33
	MOTA	1330	ND1	HIS	474	16.227	12.456	5.542	1.00	38.97
	MOTA	1331	CE1	HIS	474	15.053	11.883	5.732	1.00	37.99
	MOTA	1332	NE2	HIS	474	14.116	12.686	5.261	1.00	37.43
40	MOTA	1333	C	HIS	474	17.403	15.573	6.815	1.00	29.74
	MOTA	1334	. 0	HIS	474	16.460	15.543	7.596	1.00	29.90
	MOTA	1335	N	ILE	475	18.653	15.326	7.185	1.00	27.80
	MOTA	1336		ILE	475	18.971	15.014	8.571	1.00	25.61
	ATOM	1337		ILE	475	20.478	14.708	8.720	1.00	25.59
45	MOTA	1338		ILE	475	20.877	14.713	10.193	1.00	27.17
	ATOM	1339		ILE	475	20.787	13.341	8.092	1.00	26.17
	MOTA	1340		ILE	475	22.258	13.071	7.849		27.07
	ATOM	1341		ILE	475	18.576	16.201	9.460		27.91
~ 0	ATOM	1342		ILE	475	17.928		10.485		
50	MOTA	1343		HIS	476	18.956	17.404	9.054		
	MOTA	1344		HIS	476	18.621	18.575	9.846		
	MOTA	1349		HIS	476	19.342		9.281		
	ATOM	1346		HIS	476	20.777		9.699		
<i>-</i> -	ATOM	1347		HIS	476	21.355		10.915		
55	ATOM	1348		HIS	476	21.809		8.808		
	MOTA	1349		HIS	476	22.959		9.456		
	ATOM	1350		HIS	476	22.712		10.735		
	MOTA	135		HIS	476	17.120		9.948		
~	MOTA	135		HIS	476	16.636		10.951 8.929		
60		135		ARG		16.374				
	MOTA	135	4 CA	ARG	477	14.929	18.570	8.956	1.00	21.33

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5	ATOM	1355	CB	ARG	477	14.343	18.376	7.557		34.95
	MOTA	1356	CG	ARG	477	14.425	19.627	6.700	1.00	40.46
	MOTA	1357	CD	ARG	477	13.698	19.445	5.370	1.00	45.22
	ATOM	1358	NE	ARG	477	14.107	20.456	4.399	1.00	53.05
	ATOM	1359	CZ	ARG	477	13.647	21.705	4.376	1.00	55.89
10	MOTA	1360	NH1	ARG	477	12.756	22.106	5.274	1.00	56.17
	ATOM	1361	NH2	ARG	477	14.084	22.558	3.457	1.00	59.49
	ATOM	1362	С	ARG	477	14.310	17.582	9.931	1.00	30.70
	MOTA	1363	0	ARG	477	13.360	17.903	10.649	1.00	30.24
	MOTA	1364	N	VAL	478	14.863	16.375	9.972	1.00	29.67
15	MOTA	1365	CA	VAL	478	14.351	15.369	10.887	1.00	29.68
	ATOM	1366	CB	VAL	478	14.937	13.975	10.575	1.00	32.01
	ATOM	1367	CG1	VAL	478	14.461	12.973	11.609	1.00	32.93
	MOTA	1368	CG2	VAL	478	14.506	13.528	9.169	1.00	31.00
	MOTA	1369	С	VAL	478	14.696	15.774	12.316	1.00	29.81
20	MOTA	1370	0	VAL	478	13.860	15.677	13.220	1.00	30.25
	ATOM	1371	N	LEU	479	15.929	16.232	12.516	1.00	28.81
	MOTA	1372	CA	LEU	479	16.360	16.674	13.836	1.00	28.74
	MOTA	1373	CB	LEU	479	17.799	17.210	13.779	1.00	26.65
	MOTA	1374	CG	LEU	479	18.910	16.152	13.853	1.00	26.05
25	ATOM	1375	CD1	LEU	479	20.231	16.772	13.395	1.00	25.81
	MOTA	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.34
	ATOM	1377	С	LEU	479	15.411	17.777	14.313	1.00	29.54
	MOTA	1378	0	LEU	479	14.997	17.786	15.472	1.00	29.00
	MOTA	1379	N	ASP	480	15.076	18.703	13.415	1.00	31.52
30	MOTA	1380	CA	ASP	480	14.162	19.800	13.741	1.00	33.84
	MOTA	1381	CB	ASP	480	13.943	20.712	12.528	1.00	34.37
	MOTA	1382	CG	ASP	480	15.055	21.743	12.345	1.00	36.26
	ATOM	1383		ASP	480	15.119	22.354	11.257	1.00	36.56
	MOTA	1384	OD2	ASP	480	15.860	21.951	13.274	1.00	34.19
35	MOTA	1385		ASP	480	12.818	19.222	14.174	1.00	33.48
	MOTA	1386		ASP	480	12.186	19.724	15.105	1.00	33.89
	ATOM	,1387		LYS	481	12.379	18.161	13.498	1.00	33.90
	MOTA	1388		LYS	481	11.106	17.536	13.839	1.00	32.97 34.66
	MOTA	1389		LYS	481	10.719	16.489	12.784	1.00	33.57
40	MOTA	1390		LYS	481	11.164	16.895	15.225 15.943	1.00 1.00	35.37
	MOTA	1391		LYS	481	10.167	16.869	15.943		32.71
	ATOM		N	ILE	482	12.328	16.377	16.922	1.00	31.60
	MOTA	1393		ILE	482	12.457		17.028		
4.5	ATOM	1394		ILE	482			18.430		
45	ATOM	1395		ILE		13.877		15.995		
	MOTA	1396			482	13.697 14.978		15.908		
	MOTA	1397				12.456		17.994		
	MOTA	1398		ILE		11.946		19.097		
~ 0	ATOM	1399		ILE		13.027		17.679		
50	ATOM	1400		THR		13.027		18.644		
	ATOM	140		THR		13.022		18.109		
	MOTA	1402		THR		15.730		17.788		
	MOTA	140				13.756		19.160		
	ATOM	140				11.559		18.920		
55		140		THR		11.559				
	MOTA	140		THR ASP		10.785				
	MOTA	140		ASP ASP		9.369				
	ATOM	140		ASP ASP		8.708				
<i>د</i> ۸	MOTA	140		ASP ASP						
60		141								
	MOTA	141	1 OD1	. ASP	484	9.0/1	. 22.043	20.200		

5	ATOM	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49
	ATOM	1413	C	ASP	484	8.657	18.985	18.840	1.00	
	ATOM	1414	0	ASP	484	7.830	19.339	19.676	1.00	34.86
	ATOM	1415	N	THR	485	8.996	17.715	18.646	1.00	33.91
	ATOM	1416	CA	THR	485	8.396	16.635	19.414	1.00	34.41
10	ATOM	1417	CB	THR	485	8.875	15.268	18.885	1.00	33.58
	MOTA	1418	OG1	THR	485	8.400	15.094	17.542	1.00	
	ATOM	1419	CG2	THR	485	8.347	14.138	19.751	1.00	37.04
	MOTA	1420	С	THR	485	8.708	16.757	20.903	1.00	30.89
	ATOM	1421	0	THR	485	7.818	16.600	21.744	1.00	35.15
15	ATOM	1422	N	LEU	486	9.966	17.046	21.744		31.99
	ATOM	1423	CA	LEU	486	10.368	17.192		1.00	33.77
	ATOM	1424	CB	LEU	486	11.879	17.192	22.621	1.00	34.31
	MOTA	1425	CG	LEU	486	12.776		22.721	1.00	32.00
	ATOM	1426	CD1	LEU	486	14.233	16.201	22.754	1.00	34.99
20	ATOM	1427	CD2	LEU	486		16.613	22.521	1.00	32.65
	ATOM	1428	C	LEU	486	12.635 9.597	15.481	24.105	1.00	29.90
	ATOM	1429	0	LEU	486		18.348	23.256	1.00	34.87
	ATOM	1430	N	ILE		9.078	18.225	24.362	1.00	35.85
	ATOM	1431	CA		487	9.513	19.469	22.548	1.00	35.59
25	ATOM	1431	CB	ILE	487	8.787	20.625	23.064	1.00	36.79
23	ATOM	1432	CG2	ILE	487	8.890	21.826	22.095	1.00	37.32
	ATOM	1433		ILE	487	7.833	22.884	22.443	1.00	40.19
	MOTA	1434	CG1	ILE	487	10.292	22.443	22.181	1.00	36.00
	MOTA		CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
30	ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56
50	ATOM	1437	0	ILE	487	6.708	20.628	24.282	1.00	38.52
		1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
	MOTA MOTA	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
	ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
35	ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
55		1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
	ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
	ATOM ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
		1445	NE2	HIS	488	1.477	17,144	21.385	1.00	50.22
40	ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
40	ATOM	1447	0	HIS	488	4.233	18.498	24.467	1.00	43.02
	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	39.91
	ATOM	1449	CA	LEU	489	5.936	16.399	25.048	1.00	39.93
	ATOM	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
45	ATOM	1451	CG	LEU	489	6.961	14.242	24.056	1.00	39.31
43	ATOM	1452	CD1	LEU	489	8.259	13.456	24.027	1.00	39.01
	ATOM	1453	CD2	LEU	489	5.799	13.345	24.459	1.00	41.98
	MOTA	1454	C	LEU	489	5.973	17.203	26.339	1.00	40.24
	MOTA	1455	0	LEU	489	5.267	16.888	27.298	1.00	38.72
50	MOTA	1456	N	MET	490	6.798	18.246	26.353	1.00	39.94
50	ATOM	1457	CA	MET	490	6.939	19.102	27.522	1.00	41.50
	MOTA	1458	CB	MET	490	8.208	19.953	27.394	1.00	39.15
	MOTA	1459	CG	MET	490	9.495	19.169	27.608	1.00	41.69
	ATOM	1460	SD	MET	490	10.978	20.106	27.161	1.00	35.76
	ATOM	1461	CE	MET	490	12.178	18.775	27.056	1.00	39.22
55	ATOM	1462	C	MET	490	5.718	20.004	27.717	1.00	
	ATOM	1463	0	MET	490	5.296	20.004	28.848		42.33
	ATOM	1464	N	ALA	491	5.162	20.238	26.616	1.00	41.09
	ATOM	1465	CA	ALA	491	3.983	20.498		1.00	43.15
	ATOM	1466	CB	ALA	491	3.622	21.331	26.693	1.00	43.79
60	ATOM	1467	C	ALA	491	2.841	20.510	25.311	1.00	43.93
	ATOM		Ö	ALA	491	2.073		27.251	1.00	46.16
			-	4 3445	マノエ	4.0/3	20.967	28.095	1.00	44.69

	****	,0001							
			- 170	402	2.752	19.268	26.783 1	00 46	5.29
5	MOTA	1469 N		492	1.711			1.00 49	9.90
	MOTA	1470 CA	LYS	492 492	1.772	17.053		1.00 50	0.03
	MOTA	1471 CB	LYS		1.087	17.135		1.00 5	3.81
	MOTA	1472 CG	LYS	492	-0.002	16.084		1.00 5	9.00
	MOTA	1473 CD	LYS		-0.988	16.453		1.00 6	1.85
10	MOTA	1474 CE	LYS	492	-1.351	15.281		1.00 6	2.89
	MOTA	1475 NZ	LYS	492	1.841	18.025			1.15
	MOTA	1476 C	LYS	492		17.784			3.37
	ATOM	1477 O	LYS	492	0.845	18.012			0.15
	MOTA	1478 N	ALA	493	3.072	17.706	30.600		9.17
15	MOTA	1479 CA	ALA	493	3.321	17.700	30.794	-	0.39
	MOTA	1480 CB	ALA	493	4.777	18.885	31.501		9.36
	MOTA	1481 C	ALA	493	2.971	18.799	32.723		1.57
	MOTA	1482 O	ALA	493	3.089		30.893		8.61
	MOTA	1483 N	GLY	494	2.554	19.989	31.671		16.92
20	MOTA	1484 CA	\mathtt{GLY}	494	2.185	21.159	32.006		15.46
	MOTA	1485 C	\mathtt{GLY}	494	3.322	22.107	32.000		43.58
	MOTA	1486 O	${ t GLY}$	494	3.206	22.921	31.284		44.81
	MOTA	1487 N	LEU	495	4.431	22.009			42.34
	ATOM	1488 CA	LEU	495	5.555	22.899	31.540 30.988		43.79
25	MOTA	1489 CB	LEU	495	6.847	22.293			40.99
	MOTA	1490 CG	LEU	495	7.712	21.459	31.936 32.260		44.70
	ATOM	1491 CD	1 LEU	495	7.022	20.156	32.260		42.12
	MOTA	1492 CD	2 LEU	495	9.072	21.189			42.13
	MOTA	1493 C	FEA	495	5.278	24.227	30.847	1.00	42.49
30	MOTA	1494 0	LEU	495	4.664	24.258	29.778	1.00	42.73
. 50	MOTA	1495 N	THR	496	5.718	25.324	31.452	1.00	43.56
	MOTA	1496 CA	THR	496	5.521	26.636	30.845	1.00	46.09
	MOTA	1497 CE	THR	496	5.841	27.767	31.829	1.00	43.92
	ATOM	1498 00	THR	496	7.222		32.208 33.064	1.00	45.63
35	ATOM	1499 CC	32 THR	496	4.965			1.00	45.54
	MOTA	1500 C	THR	496	6.471			1.00	43.39
	MOTA	1501 0	THR		7.370			1.00	45.02
	MOTA	1502 N	LEU		6.280			1.00	45.12
	ATOM	1503 C	A LEU		7.135				46.62
40		1504 C	B LEU		6.710				50.20
	MOTA	1505 C			5.933				50.95
	MOTA	1506 C	D1 LEU		5.886				50.91
	MOTA	1507 C	D2 LEU		6.589				44.94
	MOTA	1508 C			8.599				45.03
45	ATOM	1509 C			9.474				41.14
	MOTA	1510 N			8.86				40.54
	MOTA	1511 C	:A GLI		10.22				43.82
	MOTA	1512	B GLI		10.24			_	43.37
	MOTA	1513	G GLI		11.58				47.03
5		1514	CD GL		11.53				49.18
_	MOTA	1515	DE1 GL		10.56				45.30
	MOTA	1516 N	TE2 GL		12.59				39.39
	ATOM		GL:		10.77				35.05
	ATOM		O GL						36.49
5	5 ATOM		4 GL	N 499					
,	MOTA		CA GL						
	MOTA		CB GL						
	MOTA		CG GL						
	ATOM	_	CD GL						
4	50 ATOM		OE1 GI						_
•	ATOM ATOM		NE2 GI	N 499	8.2	2225.10	35.82	9 1.00	Z3.70
	ALON				231				

5	MOTA	1526	C	GLN	499	10.655	24.773	30.285		35.03
	MOTA	1527	0	GLN	499	11.446	23.832	30.422	1.00	36.59
	MOTA	1528	N	GLN	500	9.980	24.994	29.162	1.00	34.14
	MOTA	1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
10	MOTA	1530	СВ	GLN	500	9.042	24.436	26.958	1.00	33.90
10	MOTA	1531	CG	GLN	500	7.672	23.872	27.315	1.00	36.62
	MOTA	1532	CD	GLN	500	6.558	24.419	26.435	1.00	40.17
	MOTA	1533	OE1	GLN	500	6.660	24.417	25.207	1.00	40.22
	MOTA	1534	NE2	GLN	500	5.482	24.886	27.064	1.00	41.82
	MOTA	1535	C	GLN	500	11.511	24.350	27.358	1.00	34.96
15	MOTA	1536	0	GLN	500	12.256	23.387	27.124	1.00	30.79
	MOTA	1537	N	HIS	501	11.835	25.612	27.078	1.00	34.21
	MOTA	1538	CA	HIS	501	13.117	25.966	26.480	1.00	37.42
	ATOM	1539	CB	HIS	501	13.195	27.476	26.246	1.00	43.08
	MOTA	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
20	MOTA	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
	MOTA	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
	MOTA	1543	CE1	HIS	501	10.325	29.337	25.037	1.00	54.36
	MOTA	1544	NE2	HIS	501	10.466	28.508	24.018	1.00	55.19
0.5	ATOM	1545	C	HIS	501	14.255	25.543	27.395	1.00	35.79
25	MOTA	1546	0	HIS	501	15.271	24.996	26.945	1.00	36.20
	MOTA	1547	N	GLN	502	14.086	25.799	28.685	1.00	33.90
	MOTA	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
	MOTA	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
20	MOTA	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
30	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
	ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
	ATOM	1554	C	GLN	502	15.340	23.932	29.716	1.00	31.79
35	ATOM	1555	0	GLN	502	16.483	23.479	29.769	1.00	28.00
33	ATOM	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
	ATOM	1557 1558	CA	ARG ARG	503 503	14.436	21.704 21.011	29.779 30.052	1.00	29.91 32.79
	MOTA MOTA	1559	CB CG	ARG	503	13.107 13.258	19.541	30.400	1.00	30.84
	MOTA	1560	CD	ARG	503	11.930	18.935	30.798	1.00	30.61
40	ATOM	1561	NE	ARG	503	12.021	17.490	30.992	1.00	28.50
	ATOM	1562	CZ	ARG	503	12.489	16.908	32.093	1.00	29.00
	ATOM		NH1	ARG	503	12.917	17.640	33.114	1.00	29.85
	ATOM	1564	NH2	ARG	503	12.512	15.583	32.180	1.00	33.73
	ATOM	1565		ARG	503	15.051	21.152	28.496	1.00	29.89
45	ATOM	1566		ARG	503	15.895	20.259	28.548	1.00	29.69
	ATOM	1567		LEU	504	14.624	21.675	27.351	1.00	28.99
	MOTA	1568	CA	LEU	504	15.164	21.223	26.075	1.00	28.90
	ATOM	1569		LEU	504	14.566	22.023	24.916	1.00	27.72
	ATOM	1570		LEU	504	15.327	21.901	23.593	1.00	30.47
50	ATOM	1571		LEU	504	15.252	20.453	23.117	1.00	31.74
	ATOM	1572		LEU	504	14.742	22.843	22.542	1.00	29.85
	ATOM	1573		LEU	504	16.681	21.419	26.089	1.00	29.69
	ATOM	1574		LEU	504	17.439	20.536	25.672	1.00	26.38
	ATOM	1575		ALA	505	17.114	22.585	26.564	1.00	28.51
55	ATOM	1576		ALA	505	18.535	22.899	26.632	1.00	25.98
-	ATOM	1577		ALA	505	18.735	24.361	27.039	1.00	29.86
	ATOM	1578		ALA	505	19.261	21.977	27.604	1.00	26.67
	ATOM	1579		ALA	505	20.340	21.462	27.290	1.00	25.54
	ATOM	1580		GLN	506	18.677	21.771	28.784	1.00	23.59
60	MOTA	1581		GLN	506	19.299	20.907	29.785	1.00	27.67
	MOTA	1582		GLN	506	18.434	20.796	31.043	1.00	27.75

5	a trom	1583	CG	GLN	506	18.414	22.027	31.945		32.48
	ATOM	1584	CD		506	17.111	22.116	32.736		38.40
•	ATOM	1585	OE1	-	506	16.319	21.167	32.754		35.97
	MOTA	1586	NE2	GLN	506	16.879	23.257	33.386	1.00	38.07
	ATOM	1587	C	GLN	506	19.500	19.509	29.217	1.00	24.53
10	ATOM	1588	0	GLN	506	20.536	18.889	29.441	1.00	26.42
10	MOTA		И	LEU	507	18.505	19.017	28.484	1.00	26.78
	ATOM	1589		LEU	507	18.578	17.678	27.902	1.00	26.18
	MOTA	1590	CA	LEU	507	17.225	17.286	27.295	1.00	31.48
•	MOTA	1591	CB		507	16.052	16.961	28.231		32.59
	MOTA	1592	CG	LEU	507	14.836	16.561	27.389	1.00	33.78
15	MOTA	1593	CD1	LEU		16.431	15.838	29.174	1.00	30.18
	MOTA	1594	CD2	LEU	507	19.652	17.583	26.819	1.00	26.03
	MOTA	1595	С	LEU	507		16.621	26.771	1.00	27.28
	MOTA	1596	0	LEU	507	20.421	18.583	25.950	1.00	24.31
	MOTA	1597	N	LEU	508	19.713		24.863	1.00	23.68
20	MOTA	1598	CA	LEU	508	20.690	18.557	23.828	1.00	23.91
	MOTA	1599	CB	LEU	508	20.339	19.629		1.00	24.68
	MOTA	1600	CG	LEU	508	19.004	19.436	23.102	1.00	25.11
	ATOM	1601	CD1	LEU	508	18.905	20.416	21.945		27.53
	MOTA	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	22.93
25	MOTA	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.33
	MOTA	1604	0	LEU	508	23.062	18.200	24.736	1.00	
	MOTA	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
	MOTA	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
	MOTA	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
30	MOTA	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
	MOTA	1609		LEU	509	23.529	23.114	28.921	1.00	35.23
	MOTA	1610		LEU	509	24.818	22.525	26.856	1.00	30.48
	ATOM	1611		LEU	509	24.154	18.327	27.540	1.00	26.08
	ATOM	1612		LEU	509	25.354	18.068	27.547	1.00	23.92
35	ATOM	1613		ILE	510	23.254	17.462	27.993	1.00	24.60
30	MOTA	1614		ILE	510	23.712	16.172	28.496	1.00	25.12
	ATOM	1615		ILE	510	22.568	15.368	29.161	1.00	28.51
	ATOM	1616		ILE	510	23.051	13.965	29.506	1.00	31.67
	ATOM	161			510	22.141	16.060	30.459	1.00	31.18
40	MOTA	161			510	20.712	15.749	30.882	1.00	37.16
40	MOTA	161		ILE	510	24.337	15.351	27.364		23.86
	MOTA	162		ILE	510	25.225	14.534	27.600	1.00	24.14
	MOTA	162		LEU	511	23.889		26.133		25.10
	ATOM	162		LEU	511	24.420	14.862	24.977		25.63
45		162		LEU	511	23.628	15.225	23.714	1.00	23.89
40	ATOM	162		LEU		22.152	14.801	23.659	1.00	25.78
	MOTA	162				21.648		22.224	1.00	26.55
		162				21.990		24.146	1.00	26.29
	MOTA	162		LEU		25.912			1.00	27.10
50	MOTA	162		LEU		26.643			1.00	24.98
50				SER		26.372			1.00	24.75
	MOTA	162		SER		27.78				23.68
	MOTA	163				28.02				_
	MOTA	163		SER		29.27	=			_
	MOTA	163		SER						_
55		163		SER		28.59				
	MOTA	163		SER		29.74				
	MOTA	163		AHĮ						
	MOTA	163		BHI						
	MOTA	163								
60	MOTA 0	163								
	MOTA	16:	39 CB	IHA	S 513	27.92	0 14.77	o 49.33	0.30	, 23.33

5	MOTA	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
	MOTA	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
	MOTA	1643	CD2	AHIS	513	29.223	16.616	30.824	0.50	27.56
10	MOTA	1644	CD2	BHIS	513	30.095	14.211	31.001	0.50	24.22
10	MOTA	1645	ND1	AHIS	513	27.204	17.117	30.160	0.50	30.62
	MOTA	1646	ND1	BHIS	513	28.285	13.105	31.523	0.50	27.00
	MOTA	1647	CE1	AHIS	513	27.693	18.185	30.763	0.50	26.32
	MOTA	1648	CE1	BHIS	513	29.225	12.740	32.376	0.50	24.40
	MOTA	1649	NE2	AHIS	513	28.916	17.908	31.176	0.50	28.30
15	MOTA	1650	NE2	BHIS	513	30.334	13.396	32.081	0.50	25.54
	ATOM	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	ATOM	1652	C	BHIS	513	28.720	13.171	27.652	0.50	19.42
	MOTA	1653	0	AHIS	513	29.601	12.426	28.026	0.50	22.45
	MOTA	1654	0	BHIS	513	29.707	12.457	27.809	0.50	22.62
20	MOTA	1655	N	ILE	514	27.633	12.753	27.015	1.00	20.76
	ATOM	1656	CA	ILE	514	27.572	11.396	26.492	1.00	20.94
	MOTA	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
	MOTA	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
	MOTA	1659	CG1	ILE	514	25.185		27.139	1.00	27.91
25	MOTA	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	MOTA	1661	C	ILE	514	28.641	11.256	25.398	1.00	20.66
	MOTA	1662	0	ILE	514	29.298	10.226	25.285	1.00	22.21
	MOTA	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
	MOTA	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
30	MOTA	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	MOTA	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
	MOTA	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55
	ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24
	MOTA	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
35	MOTA	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
	MOTA	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
	ATOM	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
	ATOM	1673	0	ARG	515	32.068	11.305	23.795	1.00	20.06
	MOTA	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
40	MOTA	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
	MOTA	1676	CB	HIS	516	32.566	13.794	27.206	1.00	24.03
	MOTA	1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
	MOTA	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
	MOTA	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
45	ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
	ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
	MOTA	1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
	MOTA	1683	0	HIS	516	34.059	10.852	26.362	1.00	23.66
	MOTA	1684	N	MET	517	31.969	10.786	27.168	1.00	20.91
50	MOTA	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
	ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
	MOTA	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
	MOTA	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
	ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
55	MOTA	1690	С	MET	517	32.399	8.448	26.564	1.00	23.26
	ATOM	1691	0	MET	517	33.213	7.547	26.728	1.00	26.08
	ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
	ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
	ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
60	ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
	ATOM	1696	С	SER	518	33.432	7.862	23.810	1.00	25.15
									2.00	ر د . د د

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5	ATOM	1697	0	SER	518	34.111	6.866	23.532	1.00	22.94
	ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	22.42
	MOTA	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
	MOTA	1700	CB	NSA	519	35.605	10.807	23.157	1.00	24.46
	MOTA	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
10	MOTA	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
	MOTA	1703	ND2	ASN	519	34.459	12.715	22.224	1.00	28.81
	MOTA	1704	С	ASN	519	36.292	8.643	24.201	1.00	21.46
	ATOM	1705	0	ASN	519	37.251	8.015	23.752	1.00	23.56
	MOTA	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.23
15	MOTA	1707	CA	LYS	520	36.964	8.171	26.488	1.00	26.35
	MOTA	1708	CB	LYS	520	36.581	8.592	27.912	1.00	27.53
	ATOM	1709	CG	LYS	520	36.618	10.101	28.174	1.00	33.74
	MOTA	1710	CD	LYS	520	37.962	10.710	27.811	1.00	42.09
	ATOM	1711	CE	LYS	520	39.047	10.307	28.802	1.00	43.97
20	ATOM	1712	NZ	LYS	520	39.858	11.480	29.254	1.00	48.07
	MOTA	1713	C	LYS	520	36.899	6.644	26.376	1.00	27.71
	MOTA	1714	0	LYS	520	37.913	5.957	26.501	1.00	27.15
	MOTA	1715	N	GLY	521	35.704	6.117	26.141	1.00	25.02
	ATOM	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
25	ATOM	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
	ATOM	1718	0	GLY	521	36.924	3.128	24.775	1.00	26.84
	MOTA	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
	MOTA	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
	ATOM	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
30	ATOM	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
	MOTA	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
	ATOM	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
	ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
	MOTA	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70
35	ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
	MOTA	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
	ATOM	1729	CE	AMET	522	33.142	4.017	19.031	0.50	31.29
	MOTA	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
	ATOM	1731	C	AMET	522	38.242	4.532	22.512	0.50	28.99
40	MOTA	1732	C	BMET	522	38.224	4.567	22.483	0.50	30.76
	ATOM	1733	0	AMET	522	38.939	3.743	21.870	0.50	31.65
	ATOM	1734	0	BMET	522	38.905	3.793	21.807	0.50	32.87
	ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
	ATOM	1736	CA	GLU	523	40.190	5.576	23.513	1.00	34.09
45	MOTA	1737		GLU	523	40.515	6.725	24.480	1.00	35.59
	MOTA	1738	CG	GLU	523	40.658	8.079	23.784	1.00	43.35
	MOTA	1739		GLU	523	40.560	9.265	24.739	1.00	46.63
	MOTA	1740			523	39.832	10.240	24.416	1.00	47.64
	MOTA	1741			523	41.212	9.225	25.805	1.00	43.09
50	MOTA	1742		GLU	523	40.718	4.260	24.061	1.00	34.62
	MOTA	1743	0	GLU	523	41.733	3.747	23.596	1.00	33.87
	MOTA	1744		HIS	524	40.021	3.700	25.042	1.00	36.33
	ATOM	1745		HIS	524	40.455	2.427	25.607	1.00	39.20
	MOTA	1746		HIS	524	39.678	2.093	26.878	1.00	40.75
55	ATOM	1747		HIS	524	40.061	0.774	27.473	1.00	48.10
	ATOM	1748			524	41.192	0.376	28.104	1.00	48.56
	ATOM	1749			524		-0.338	27.412	1.00	48.84
	MOTA	1750			524		-1.362	27.978	1.00	50.19
	MOTA	1751			524		-0.956	28.407	1.00	51.61
60	ATOM	1752		HIS	524		1.282	24.613	1.00	38.06
	ATOM	1753		HIS	524		0.521	24.371	1.00	38.18
		_,	_				0.521	22.7/1	1.00	20.10

5	ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
	MOTA	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
	ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
	ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
	ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
10	MOTA	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
	MOTA	1760	С	LEU	525	39.859	0.057	21.954	1.00	41.32
	ATOM	1761	0	LEU	525	40.244	-1.015	21.487	1.00	40.76
	ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
	MOTA	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00
15	MOTA	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
	MOTA	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
	MOTA	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	ATOM	1767	CE1	TYR	526	42.681	2.875	16.305	1.00	61.21
	ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
20	MOTA	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
	ATOM	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
	MOTA	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	MOTA	1772	С	TYR	526	42.671	0.871	20.964	1.00	50.14
	MOTA	1773	0	TYR	526	43.471	0.303	20.223	1.00	50.73
25	MOTA	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
	MOTA	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
	MOTA	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	MOTA	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
	ATOM	1778	С	SER	527	44.365	-0.718	23.054	1.00	60.39
30	MOTA	1779	0	SER	527	45.398	-1.185	23.534	1.00	60.43
	MOTA	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
	MOTA	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	ATOM	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
	MOTA	1783	CG	MET	528	41.237	-2.606	24.222	1.00	70.10
35	MOTA	1784	SD	MET	528	39.895	-3.569	24.983	1.00	71.70
	MOTA	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
	ATOM	1786	C	MET	5,28	42.726	-3.502	21.513	1.00	70.33
	MOTA	1787	0	MET	528	42.170	-4.602	21.513	1.00	72.43
40	MOTA	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
40	MOTA	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	MOTA	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
	MOTA	1791		LYS	529	42.813	-4.439	18.587		72.47
	MOTA	1792		LYS	529	43.990	-4.762	18.751	1.00	70.37
45	MOTA	1793		CYS	530	41.932	-5.191	17.930	1.00	74.48
45	ATOM	1794		CYS	530	42.279	-6.474	17.325	1.00	76.67
	ATOM	1795		CYS	530	41.004	-7.245	16.952	1.00	77.23
	ATOM	1796		CYS	530	40.447	-8.491	18.146	1.00	79.38
	ATOM	1797		CYS	530	43.098	-6.220	16.065	1.00	78.08
50	ATOM	1798		CYS	530	43.241	-5.076	15.623	1.00	78.81
50	MOTA	1799		LYS	531	43.637	-7.289	15.487	1.00	78.22
	MOTA	1800		LYS	531	44.424	-7.187	14.267	1.00	78.15
	ATOM	1801		LYS	531	45.600	-8.182	14.305	1.00	78.33
	MOTA	1802		LYS	531	43.508	-7.467	13.067	1.00	77.93
<i>E E</i>	ATOM	1803		LYS	531	42.549	-6.734	12.839	1.00	78.07
55	ATOM	1804		ASN	532	43.784	-8.539	12.328	1.00	77.80
	ATOM	1805		ASN	532	42.984	-8.902	11.152	1.00	77.30
	ATOM	1806		ASN	532	43.550	-10.166	10.521	1.00	77.55
	ATOM	1807		ASN	532	41.485	-9.082	11.423	1.00	77.34
~	ATOM	1808		ASN	532	40.904	-10.123	11.118	1.00	78.13
60	ATOM	1809		VAL	533	40.859	-8.055	11.988	1.00	76.13
	MOTA	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77

5	ATOM	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62
	ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
	MOTA	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
	MOTA	1814	C	VAL	533	38.685	-7.143	11.352	1.00	72.97
	ATOM	1815	0	VAL	533	39.024	-5.960	11.252	1.00	73.91
10	MOTA	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
	MOTA	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
	MOTA	1818	CB	VAL	534	35.619	-7.646	9.328	1.00	67.32
	MOTA	1819	С	VAL	534	36.463	-5.541	10.393	1.00	63.87
	MOTA	1820	0	VAL	534	35.895	-5.519	11.486	1.00	63.55
15	ATOM	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
	MOTA	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
	MOTA	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
	MOTA	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	MOTA	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
20	MOTA	1826	C	PRO	535	34.944	-2.902	10.571	1.00	52.90
	ATOM	1827	0	PRO	535	34.067	-3.461	9.908	1.00	52.01
	MOTA	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
	MOTA	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	ATOM	1830	CB	LEU	536	33.280	·-0.796	13.128	1.00	44.35
25	MOTA	1831	CG	LEU	536	32.267	-0.911	14.273	1.00	43.48
	ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
	ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
	MOTA	1834	C	LEU	536	32.434	-1.433	10.871	1.00	43.58
	MOTA	1835	0	LEU	536	31.287	-1.862	10.734	1.00	42.14
30	ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
•	MOTA	1837	CA	TYR	537	32.269	-0.066	8.866	1.00	43.34
	MOTA	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
	MOTA	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	MOTA	1840	CD1	TYR	53 <i>7</i>	32.190	0.964	5.687	1.00	48.46
35	MOTA	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
	ATOM	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99
	MOTA	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
	MOTA	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
	MOTA	1845	OH	TYR	537	30.401	3.648	3.952	1.00	55.90
40	MOTA	1846	C	TYR	537	31.683	-1.199	8.032	1.00	43.15
	ATOM	1847	0	TYR	537	30.500	-1.191	7.696	1.00	41.54
	ATOM	1848		ASP	538	32.521	-2.175	7.702	1.00	44.67
	MOTA	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
	MOTA	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
45	ATOM	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
	MOTA	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	MOTA	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
	ATOM	1854	C	ASP	538	31.071	-4.195	7.587	1.00	43.48
	MOTA	1855	0	ASP	538	30.177	-4.738	6.940	1.00	43.95
50	MOTA	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
	ATOM	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	MOTA	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11
~ ~	MOTA	1860	CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
55	MOTA	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
	ATOM	1862	C	LEU	539	28.891	-4.451	9.651	1.00	36.38
	ATOM	1863	0	LEU	53 <i>9</i>		-5.070	9.436	1.00	35.74
	MOTA	1864	И	LEU	540	28.919	-3.146	9.894	1.00	35.50
	MOTA	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
60	ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
	MOTA	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28

	5		186	8 CD1	LEU	540	27.52	6 -1.299	12.645		
		MOTA	186	9 CD2	LEU	540	29.11				
		ATOM	187	0 C	LEU		27.06		11.985		
		ATOM	187	1 0	LEU		25.84		8.510		
		ATOM	187	2 N	LEU		27.89		8.371		
	10	ATOM	187		LEU				7.483		37.01
		ATOM	187		LEU		27.41		6.101		38.51
		ATOM	187				28.59		5.145	1.00	
		ATOM	187		LEU		28.30		3.643		
		ATOM				541	27.184		3.348		
	15		187			541	29.572	2 -1.716	2.908		44.18
	13	ATOM	187		LEU	541	26.723	3 -3.676	5.833		
		ATOM	187		LEU	541	25.616		5.297		39.75
		MOTA	1880	N C	GLU	542	27.366				36.48
		MOTA	1883	L CA	GLU	542	26.790		6.230		40.88
		MOTA	1882	2 CB	GLU	542	27.719		6.037		41.89
	20	MOTA	1883		GLU	542	27.010		6.620		44.11
		ATOM	1884		GLU	542		,	7.052		50.60
		ATOM	1885		GLU		26.434		5.887	1.00	55.80
		ATOM	1886			542	25.570		6.130	1.00	58.81
		ATOM	1887		GLU	542	26.842		4.728	1.00	57.19
	25	ATOM			GLU	542	25.414		6.691	1.00	41.58
	20		1888		GLU	542	24.472	-6.720	6.102	1.00	42.82
		ATOM	1889		MET	543	25.298		7.915	1.00	
		ATOM	1890		MET	543	24.036	-5.731	8.634	1.00	40.09
		ATOM	1891		MET	543	24.270		10.111		36.43
	20	ATOM	1892	CG	MET	543	25.137		10.808	1.00	39.95
	30	ATOM	1893	SD	MET	543	24.918			1.00	41.95
		ATOM	1894	CE	MET	543	25.324		12.604	1.00	47.17
		ATOM	1895	С	MET	543	23.001		12.964	1.00	40.88
		MOTA	1896	0	MET	543	21.808		8.072	1.00	35.02
		MOTA	1897		LEU	544			8.048	1.00	35.31
	35	ATOM	1898		LEU	544	23.457		7.629	1.00	32.90
		ATOM	1899		LEU		22.559	-2.603	7.074	1.00	36.88
		ATOM	1900	CG	LEU	544	23.225	-1.226	7.111	1.00	34.51
		ATOM	1901	CD1		544	23.268	-0.562	8.490	1.00	31.94
		ATOM	1902		LEU	544	24.284	0.564	8.478	1.00	32.27
	40	ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
		ATOM		C	LEU	544	22.148	-2.941	5.640	1.00	38.94
			1904	0	LEU	544	20.971	-2.842	5.294	1.00	39.52
		ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
		ATOM	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	
	45	ATOM	1907	CB	ASP	545	24.159	-3.780	2.620		40.78
	45	ATOM	1908	CG	ASP	545	23.922	-3.937		1.00	37.75
		ATOM	1909	OD1	ASP	545	24.881	-4.265	1.120	1.00	35.19
		ATOM	1910	OD2	ASP	545	22.768		0.380	1.00	33.48
		ATOM	1911	С	ASP	545	22.116	-3.734	0.691	1.00	31.33
		ATOM	1912	0	ASP	545		-5.015	3.349	1.00	42.87
	50	ATOM	1913	N	ALA		22.681	-6.030	2.929	1.00	44.32
		ATOM	1914	CA		546	20.853	-5.009	3.755	1.00	43.49
		ATOM	1915		ALA	546	20.069	-6.229	3.746		46.96
		ATOM		CB	ALA	546	19.213	-6.305	5.006		47.82
			1916	С	ALA	546	19.193	-6.362	2.508		
	5 5	ATOM	1917	0	ALA	546	18.804	-5.368	1.883		49.55
	<i>JJ</i>	ATOM	1918	N	HIS	547	18.895	-7.606	2.152		48.75
		ATOM	1919	CA	HIS	547	18.042	-7.884			50.98
		ATOM	1920	CB	HIS	547	18.431	-9.223	1.006		53.77
		ATOM	1921	CG	HIS	547			0.369		52.69
		ATOM	1922	CD2	HIS	547		-10.382	1.317		55.05
(60	ATOM	1923	ND1	HIS	547	17.477	-10.752			53.94
		ATOM	1924	CE1	HIS	547	19.395	-11.329		1.00	56.23
			_		*****	J4 /	19.095	-12.232	2.286		55.36

_	n m 011	1925	NE2	HIS	547		11.906			7.01
5		1925	C	HIS	547		-7.936			5.69
		1927	0	HIS	547	16.362	-7.796			1.30 7.00
		1928	N	ARG	548	15.653	-8.139			7.00 0.65
		1929	CA	ARG	548	14.245	-8.212	• •		2.69
10	ATOM	1930	CB	ARG	548	13.432	-7.171	• •		
10	MOTA	1931	CG	ARG	548	14.272				7.54
	ATOM	1932	CD	ARG	548	13.448	J			1.92
	ATOM	1933	NE	ARG	548	13.702	J	-	_	6.95
	MOTA	1934	CZ	ARG	548	14.864	• •			9.04
15	MOTA	1935	NH1	ARG	548	15.891	-3.644			0.66 0.39
13	MOTA	1936	NH2	ARG	548	15.001	-2.063			1.65
	ATOM	1937	C	ARG	548	13.695	-9.608	-	_	2.05
	MOTA	1938	0	ARG	548	12.500	-9.781			52.05 52.39
	MOTA	1939	И	LEU	549	14.576	-10.603	0.756		54.02
20	ATOM	1940	CA	LEU	549	14.188	-11.985	0.507		52.14
20	MOTA	1941	CB	LEU	549	15.433	-12.828	0.195		50.76
	MOTA	1942		LEU	549	16.461	-12.191	-0.753		50.76 57.77
	ATOM	1943		LEU	549	17.699	-13.074	-0.878		58.38
	ATOM	1944		LEU	549	15.823	-11.972	-2.108		66.65
25	ATOM	1945		LEU	549	13.431	-12.574	1.702		67.15
23	MOTA	1946		LEU	549	12.759	-13.600	1.577		67.72
	ATOM	1947		HIS	550	13.541	-11.920	2.856		69.93
	ATOM	1948		HIS	550	12.858	-12.378	4.065		70.76
	MOTA	1949		HIS	550	13.753	-12.190	5.298		71.50
30	MOTA	1950	CG	HIS	550	14.977	-13.054	5.306 4.341	1.00	71.63
5.0	MOTA	195	L CD2	HIS	550	15.539	-13.821	6.411	1.00	71.98
	MOTA	195	2 ND1	HIS	550	15.793		6.126	1.00	72.04
	ATOM	195	3 CE1			16.805		4.876	1.00	71.39
	MOTA	195	4 NE2			16.674		4.275	1.00	71.15
35	MOTA	195	5 C	HIS		11.556		5.340	1.00	70.66
	MOTA	195	6 0	HIS		10.940		3.258	1.00	72.22
	MOTA	195	7 N	ALA		11.143 9.919		3.338	1.00	73.58
	MOTA	195		ALA		9.919		2.221	1.00	73.21
	MOTA	195		ALA		8.658		3.266	1.00	74.69
40	MOTA	196		ALA		7.684		2.621	1.00	76.12
	ATOM	196		ALA		8.651		3.852		73.79
	MOTA	196				30.583		29.471		26.84
	HETATM					30.71	_	29.358		22.85
	HETATM					31.36		28.037		25.56
45										27.51
	HETAT				_				1.00	28.35
	HETAT				_					30.39
	HETAT									30.23
_	HETAT			=						31.45
50									1.00	27.93
	HETAT		71 C							24.41
	HETAT		72 C							24.26
	HETAT		73 C						1.00	25.92
_	HETAT		74 C							26.32
5	5 HETAT		75 C	_					3 1.00	29.02
	HETAT		76 C						6 1.00	28.42
	HETAT		77 0	·					0 1.00	
	HETAT		78 C	-	IT 60					
_	HETAT			-	HT 60			2 25.94		
ϵ	60 HETAT		_	_	HT 60				1 1.00	26.77
	HETAT	IN IS	981 C	0,						
						239				

5	HETATM	1982			600	33.166	-3.052	25.072	1.00	27.50
	HETATM	1983			600	32.676		23.786		
	HETATM	1984	020	OHT	600	33.206		22.795		
	HETATM	1985	C23	OHT	600	33.009		21.448		
	HETATM	1986	C24	OHT	600	34.226		20.575		_
10	HETATM	1987	N24	OHT	600	34.141		20.203	1.00	
	HETATM	1988	C25	OHT	600	33.375		18.933	1.00	
	HETATM	1989	C26	OHT	600	35.495	-5.459	20.004		
	HETATM	1990	C21	OHT	600	31.540	-2.005	23.558		
	HETATM	1991	C22	OHT	600	30.892	-1.450	24.645	1.00	
15	HETATM	1992		нон	1	20.714	-12.010		1.00	27.92
	HETATM	1993		нон	2	22.563	-0.070	23.057	1.00	27.20
	HETATM	1994		НОН	3	25.183		25.819	1.00	25.77
	HETATM	1995		нон	4	35.158	19.202	23.149	1.00	42.52
	HETATM	1956		нон	5	22.116	5.823	37.390	1.00	33.92
20	HETATM	1997		нон	6		-9.922	18.914	1.00	30.18
	HETATM	1998	01	НОН	7	29.812	6.536	19.652	1.00	26.11
	HETATM	1999	01	НОН		13.362	4.463	20.376	1.00	29.40
	HETATM	2000	01		8	19.799	-11.295	20.187	1.00	28.70
	HETATM	2000	01	HOH	9	21.205	1.466	23.794	1.00	22.47
25	HETATM	2001	01	HOH	10	21.177	-4.961	29.066	1.00	33.00
	HETATM	2002	01	НОН	11	18.591	1.863	20.518	1.00	32.59
	HETATM	2003		HOH	12	16.298	21.566	15.992	1.00	33.42
	HETATM		01	НОН	13	18.611	1.976	24.494	1.00	29.70
	HETATM	2005	01	HOH	14	38.009	8.910	21.156	1.00	39.92
30	HETATM	2006	01	НОН	15	26.549	11.664	18.080	1.00	30.25
50	HETATM	2007	01	HOH	16	20.282	-4.239	26.512	1.00	32.70
		2008	01	HOH	17	32.858	8.754	20.237	1.00	29.88
	HETATM	2009	01	нон	18	8.497	16.136	29.934	1.00	46.80
	HETATM	2010	01	HOH	19	21.940	19.301	31.632	1.00	35.72
35	HETATM	2011	01	HOH	20	35.153	2.682	14.122	1.00	41.02
33	HETATM	2012	01	HOH	21	20.358	-2.268	21.013	1.00	29.43
	HETATM	2013	01	HOH	22	35.562	10.036	36.334	1.00	41.37
	HETATM	2014	01	HOH	23	17.248	18.187	17.571	1.00	33.96
	HETATM	2015	01	HOH	24	18.445	20.973	12.346	1.00	43.44
40	HETATM	2016	01	HOH	25	12.152	23.054	33.132	1.00	36.04
40	HETATM	2017	01	HOH	26	13.181	22.222	9.699	1.00	37.03
	HETATM	2018	01	HOH	27	19.399	-6.090	12.808	1.00	44.86
	HETATM	2019	01	HOH	28	37.895	13.599	31.395	1.00	47.26
	HETATM	2020	01	HOH	29	11.570	6.212	7.962	1.00	51.10
4 ~	HETATM	2021	01	HOH	30	20.172	-2.568	23.445	1.00	51.70
45	HETATM	2022	01	HOH	31	36.402	-5.369	23.729	1.00	58.20
	HETATM	2023	01	HOH	32	25.127	13.802	19.187	1.00	
	HETATM	2024	01	HOH	33	23.181	4.937	38.538	1.00	35.29 33.77
	HETATM	2025	01	HOH	34	20.550	0.421	21.276	1.00	
	HETATM	2026	01	HOH	35	39.599	13.954	27.312		29.12
50	HETATM	2027	01	HOH	36	26.445	13.863	21.285	1.00	44.08
	HETATM	2028	01	нон	37	13.759	5.079		1.00	34.97
	HETATM	2029	01	нон	38	14.150	24.731	9.108	1.00	38.54
	HETATM	2030	01	нон	39	21.060		34.529	1.00	49.72
	HETATM	2031	01	нон	40		13.886	-6.319	1.00	59.79
55	HETATM	2032	01	нон	41	32.215	6.217	8.726	1.00	60.22
	HETATM	2032	01	нон		35.105	15.704	9.069	1.00	45.15
	HETATM	2034	01		42	11.427	19.451	9.903	1.00	38.56
	HETATM	2035		HOH	43	19.662	23.472	10.333	1.00	47.71
	HETATM	2035	01	HOH	44	9.231	3.690	12.337	1.00	45.98
60	HETATM		01	НОН	45	15.313	-6.036	17.192	1.00	39.07
	HETATM	2037	01	нон	46	15.517	-3.266	17.907	1.00	37.67
	TWIIV	2038	01	HOH	47	28.784	-16.713	25.163	1.00	55.44

5	HETATM HETATM HETATM HETATM HETATM HETATM HETATM	2039 2040 2041 2042 2043 2044 2045	01 01 01 01 01 01	HOH HOH HOH HOH HOH	48 49 50 51 52 53	6.955	-10.898 13.568 -15.030 31.002 12.385 6.444 -2.048	28.271 28.233 28.603 30.284 15.164 14.452 25.518	1.00 1.00 1.00 1.00 1.00	31.27 48.83 36.91 46.73 51.17 50.38 52.29
•	HETATM HETATM HETATM	2046 2047 2048	01 01 01	нон нон	55 56 57	28.188 35.275 37.771	-15.195 -10.556 -9.103 -3.039	38.996 38.061 34.605 17.983	1.00 1.00 1.00	55.22 57.39 54.17 46.80
15	HETATM HETATM HETATM HETATM	2049 2050 2051 2052	01 01 01	HOH HOH HOH	58 59 60 61 62	31.403 30.455 25.985 35.679 14.741	-3.039 -6.352 8.255 0.749 4.029	17.005 0.416 10.462 33.936	1.00 1.00 1.00	47.05 43.32 42.99 49.59
20	HETATM HETATM HETATM HETATM	2053 2054 2055 2056	01 01	HOH HOH HOH	63 64 65 66	16.333 23.809 27.012 25.956	2.592 7.186 -1.948 -6.422	35.952 39.798 46.995 42.144	1.00 1.00 1.00	45.13 45.36 63.39 44.94
25	HETATM HETATM HETATM HETATM HETATM	2057 2058 2059 2060 2061	01 01 01	HOH HOH HOH HOH	67 68 69	23.510 41.475 36.519 30.111	-8.414 0.971 8.863	39.036 33.110 38.836 12.793	1.00 1.00 1.00	39.06 55.50 41.56 44.58
30	HETATM HETATM HETATM HETATM HETATM HETATM	2062 2063 2064 2065	2 01 3 01 4 01 5 01	HOH HOH HOH HOH	71 72 73 74 75	26.850 20.448 33.896 16.884 18.595	-3.169 3.047 0.446 0.296	1.594 1.055 16.172 26.043 27.866		
35	HETATM HETATM HETATM HETATM END	206 206	8 01 9 01	нон нон нон	76 77 78 79	6.166 18.484 1.985 12.729	20.060 23.265	19.124 16.232 29.187 27.530	1.00 1.00	35.52 46.42

5 WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

identifying a test compound that modulates coactivator binding to said nuclear receptor.

- 2. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.
- 3. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.
- 25 4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
 - 5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
 - 6. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

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PCT/US99/06899 WO 99/060014

7. The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.

- The method of claim 1, wherein said nuclear receptor coactivator binding site 8. comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 10 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
- 9. 15 The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.
 - The method of claim 1, wherein said screening is in vitro. 10.
- 20 11. The method of claim 10, wherein said screening is high throughput screening.
 - 12. The method of claim 1, wherein said assay is a biological assay.
 - 13. The method of claim 1, wherein said test compound is from a library of compounds.

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- 14. The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.
- 15. The method of claim 14, wherein said test compound is a small organic molecule, a 30 peptide, or peptidomimetic.
 - 16. The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.
- 35 17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

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- 18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 19. The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.
- 25 20. The machine readable storage medium of claim 19, wherein said thyroid receptor is human.
 - 21. The machine readable storage medium of claim 20, wherein said molecule is peptide
- The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.
 - 23. The machine-readable data storage medium according to claim 18, wherein saic molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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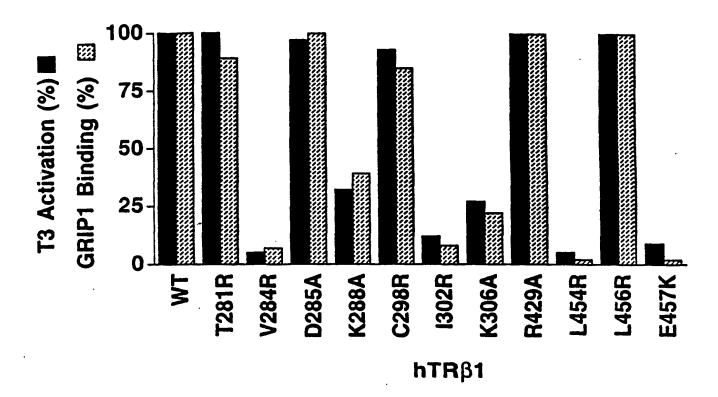
24. A machine-readable data storage medium comprising a data storage materia encoded with a first set of machine readable data which, when combined with a second set o machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises:

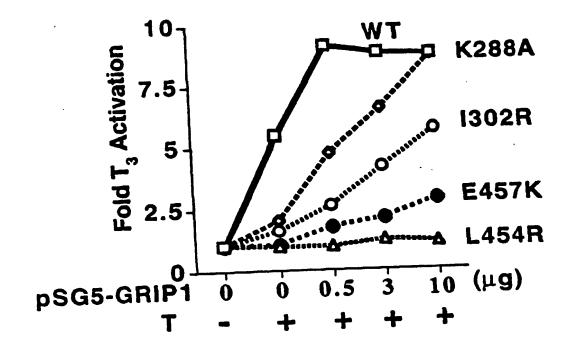
10 Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

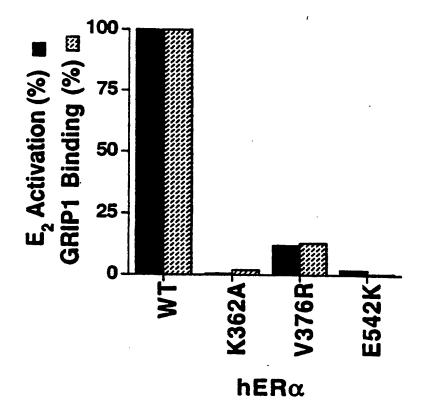
- 25. A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.
 - 26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.
 - 27. The cocrystal of claim 26, wherein said thyroid receptor is human.
 - 28. The cocrystal of claim 27, wherein said molecule is peptide.
 - 29. The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.
 - 30. A compound identified according to the method of claim 1.

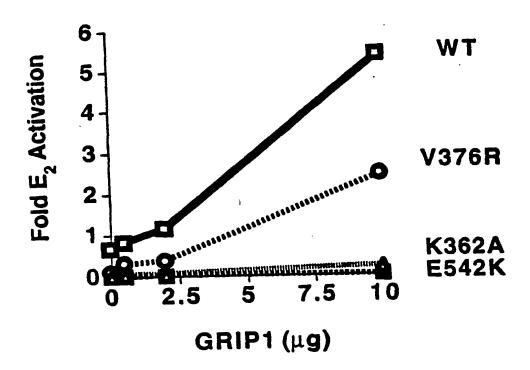
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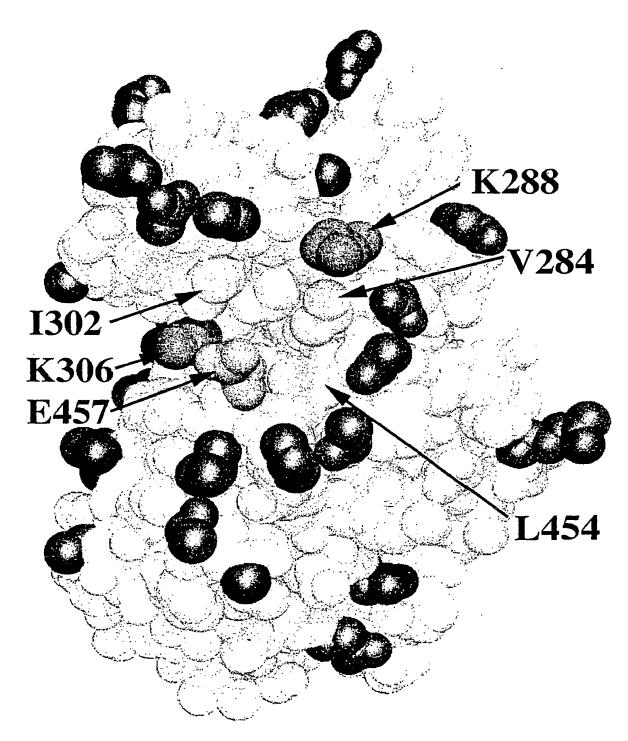


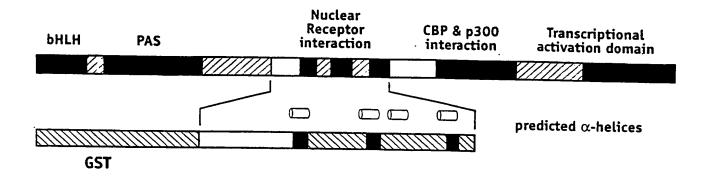
FIG. 5

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Nuclear Receptor CBP & p300 **bHLH** PAS interaction interaction Transcriptional activation domain 2 3 SEQ ID NO: 5 Gripl AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS Tif2 SEQ ID NO: 8 ADGQSRLHDSKGQTKLLQLLTTKSEOMEPSPLAS SEQ ID NO: 11 NcoA-2 AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLPS SEQ ID NO: 14 RAC3 AENQRGPLESKGHKKLLQLLTCSSEDRGHSSLTN 1 SEQ ID NO: 17 AIB1, TRAM-1 AENQRGPLESKGHKKLLQLLTCSSDDRGHSSLTN SEQ ID NO: 20 p/CIP SETPRGPLESKGHKKLLQLLTCSSEDRGHSSLTN SEQ ID NO: 23 SRC1 SEGDSKY--SQTSHKLVQLLTTTAEQQLRHADID SEQ ID NO: 26 Consensus .-....S....KLhQLLT...-.... SEQ ID NO: 6 Grip1 **PGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA** SEQ ID NO: 9 Tif2 SGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA SEQ ID NO: 12 NcoA-2 PGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA SEQ ID NO: 15 RAC3 TSNMHGSLLQEKHRILHKLLQNGNSPAEVAKITA 2 SEQ ID NO: 18 AIB1, TRAM-1 TSNMHGSLLQEKHRILHKLLQNGNSPAEVAKITA SEQ ID NO: 21 p/CIP TSNVHGSLLQEKHRILHKLLQNGNSPAEVAKITA SEQ ID NO: 24 SRC1 TCPSSHSSLTERHKILHRLLQE.GSPSDITTLSV SEQ ID NO: 27 ConsensusL.E+H+ILH+LLQ...SP.-h..h.. SEQ ID NO: 7 Gripl EPASPKKKE---NALLRYLLDKDDTKDIGLPEIT SEQ ID NO: 10 Tif2 EPVSPKKKE---NALLRYLLDKDDTKDIGLPEIT SEQ ID NO: 13 NcoA-2 EPASPKKKE---NALLRYLLDKDDTKDIGLPSIT SEQ ID NO: 16 RAC3 EQLSPKKKE--NNALLRYLLDRDDPSDVLAKKLQ 3 SEQ ID NO: 19 AIB1, TRAM-1 EQLSPKKKE--NNALLRYLLDRDDPSDALSKELQ SEQ ID NO: 22 p/CIP EQLSPKKKE--NNALLRYLLDRDDPSDALSKELQ SEQ ID NO: 25 SRC1 ELDAAKKKESKDHQLLRYLLDKDEKDLRSTPNLC SEQ ID NO: 28 Consensus E....KKKE.....LLRYLLD+D-....h. Overall Consensus (SEQ ID NO: 1)

.....LXXLL.....

FIGURE 7a



	NR-box1	NR-box1	NR box3
	residues 15-21	residues 15-21	residues 15-21
	SEQ ID NO: 5	SEQ ID NO: 6	SEQ ID NO: 7
NRb 1,2,3 NRb 1,2 NRb 1,3 NRb 1	KLLQLLT	.ILHRLLQ	.AARAAAD .LLRYLLD

FIGURE 7b

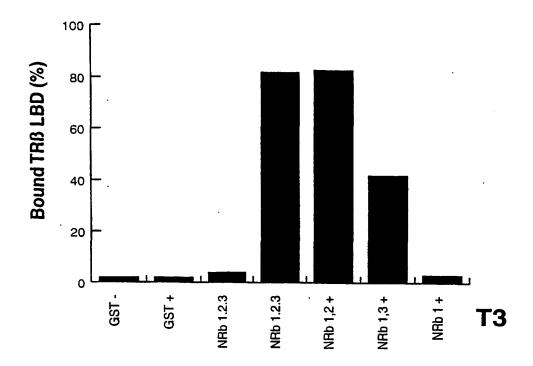
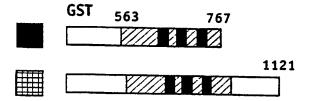


FIGURE 8a



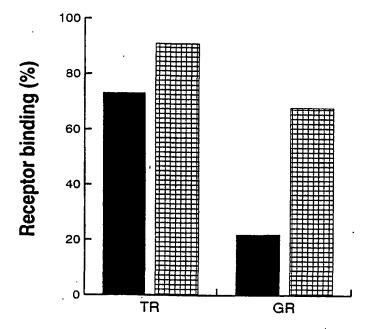
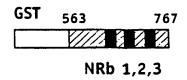
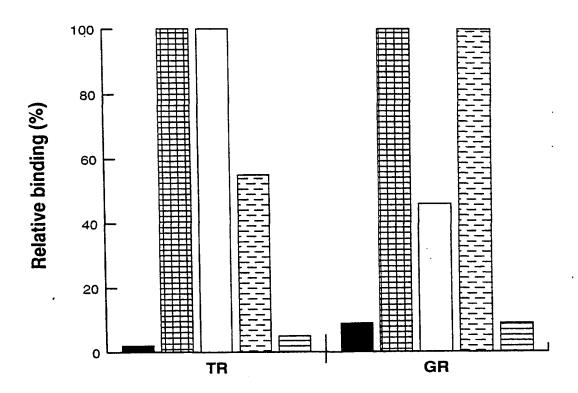


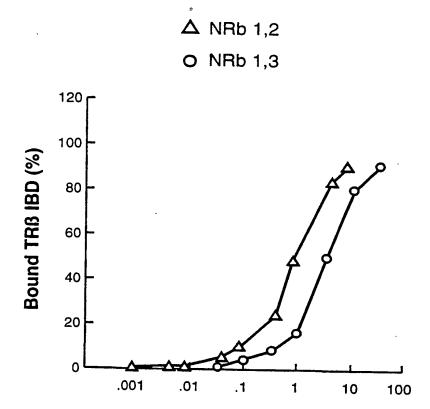
FIGURE 8b



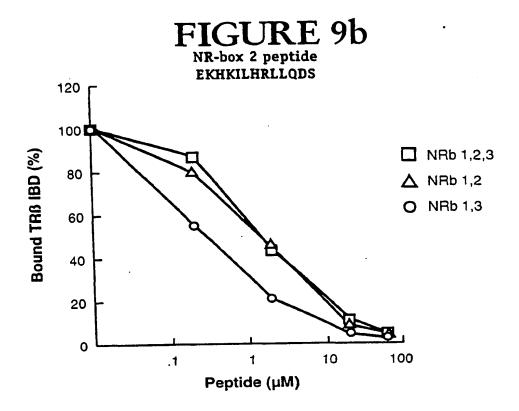


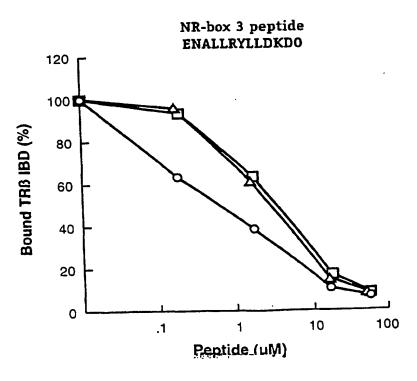
NRb 1 NRb1,3 NRb 1,2 NRb 1,2,3 GST

FIGURE 9a



NR interaction domain (µM)

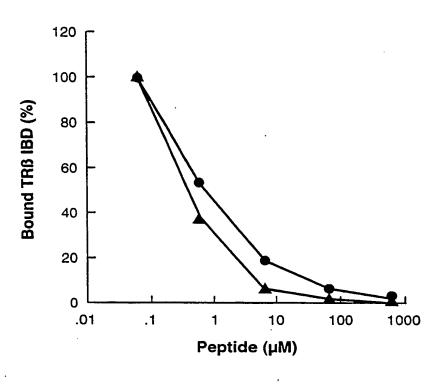




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FIGURE 10a

NR-box 2



residues 11-23residues 7-24

EKHK TSLKEKHK ILHRL ILHRL

QDS QDSS

of SEQ ID No: 6

FIGURE 10b



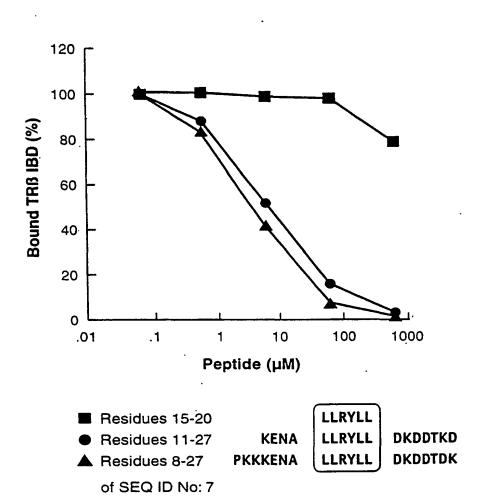
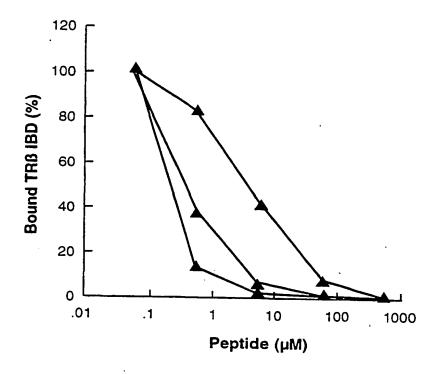


FIGURE 10c



A Residues 8027 of SEQ ID No: 7

Residues 11-27 of SEQ ID No: 6

SEQ ID No: 29

TSLKEKHK

LLRYLL

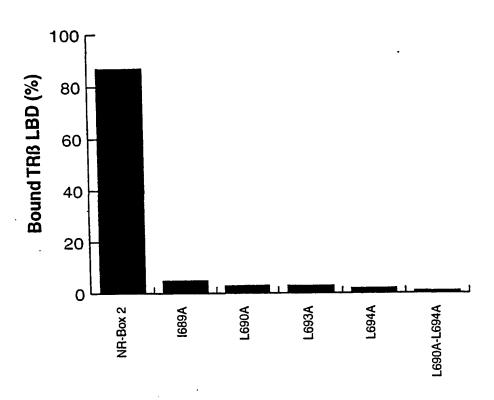
QDSS

TSLKEKHK

LLRYLL

QDSS

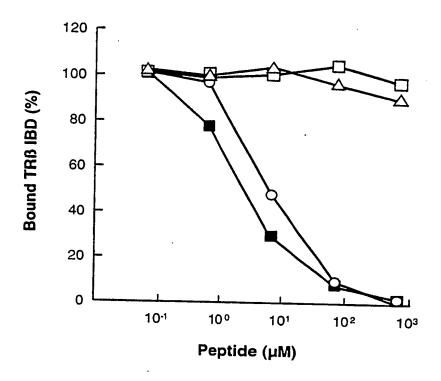
FIGURE 11a



NR-interaction domain:

NRb 1,2	ILHRLL
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L690A	IAHRLL
L693A	ILHRAL
L694A	ILHRLA
L690A/L694A	IAHRLA

FIGURE 11b



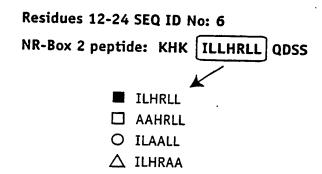
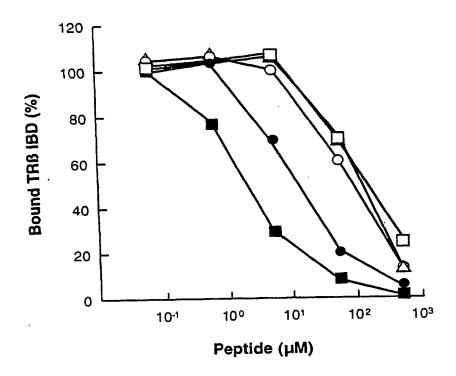
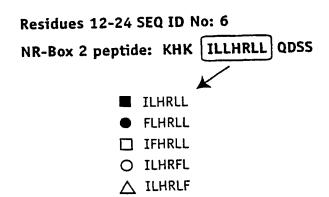
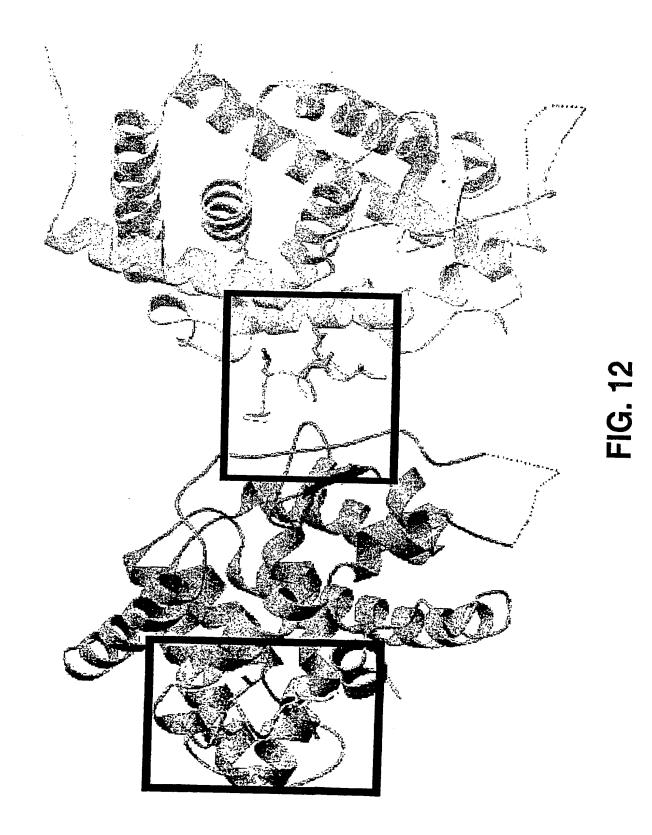


FIGURE 11c







SUBSTITUTE SHEET (RULE 26)

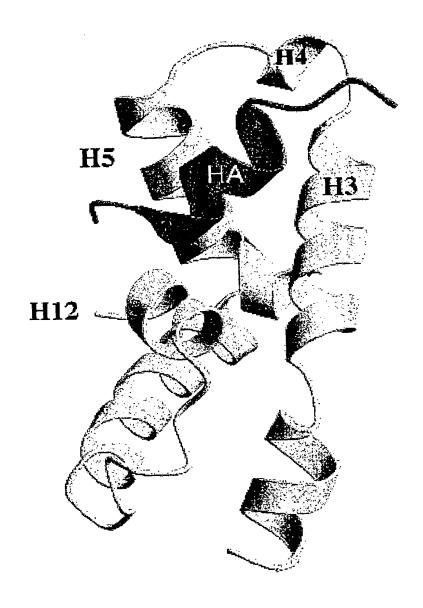


FIG. 13

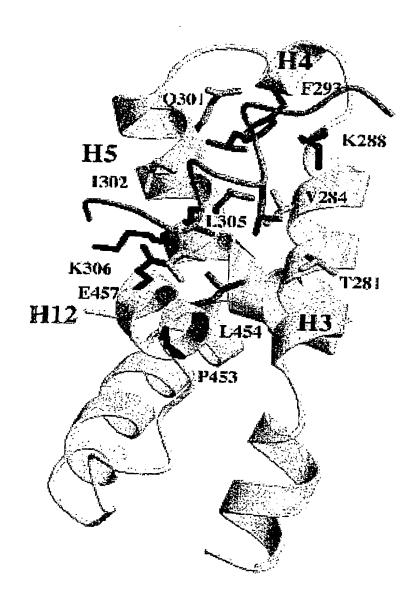


FIG. 14

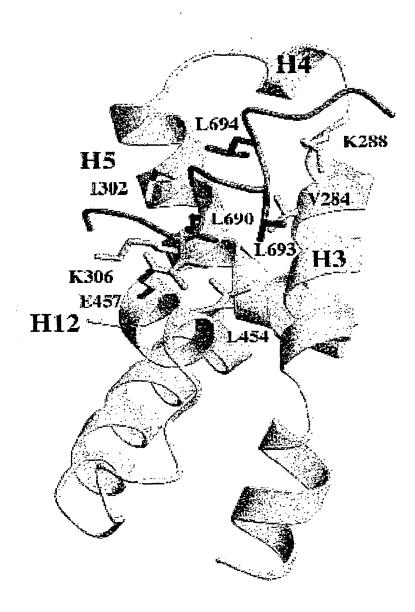


FIG. 15

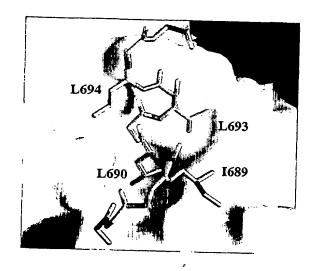


FIG. 16

SUBSTITUTE SHEET (RULE 26)

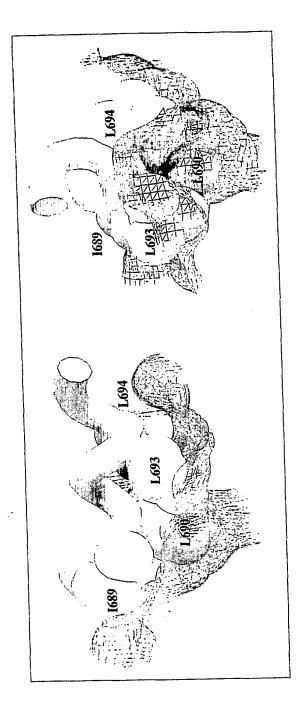


FIG. 17

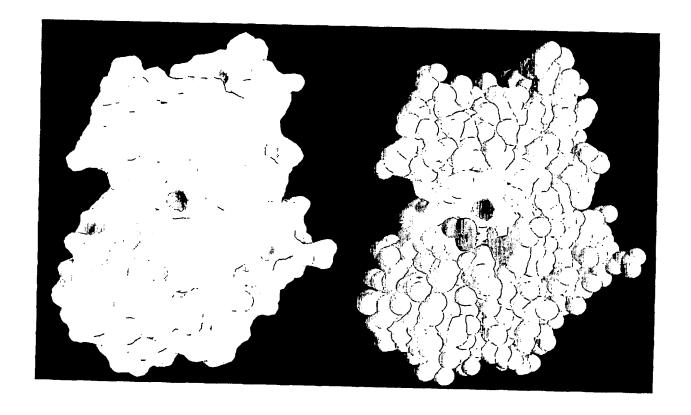
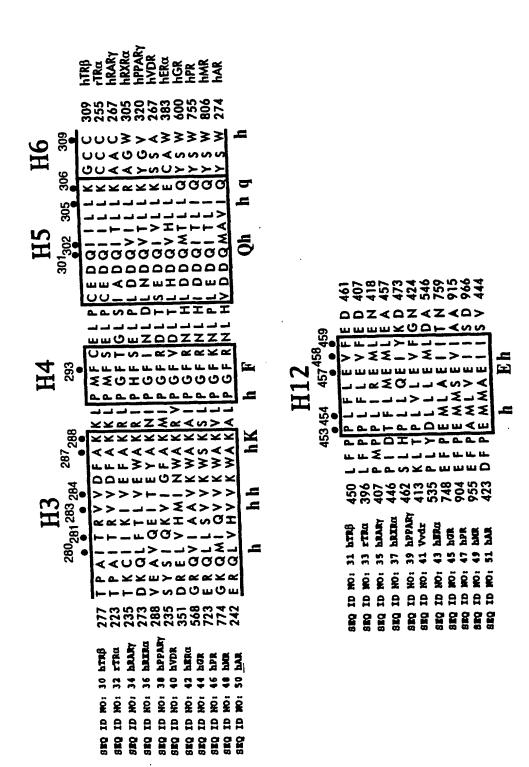


FIG. 18

SUBSTITUTE SHEET (RULE 26)





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PCT/US99/06899 WO 99/060014

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INTERNATIONAL SEARCH REPORT

PCT/US99/06899

- CLAS	SIFICATION OF SUBJECT MATTER		
	GOIN 33/50		
US CL :4	135/7.1 International Patent Classification (IPC) or to both national	onal classification and IPC	
RIELL	OS SEARCHED		
inimum do	cumentation searched (classification system followed by	classification symbols)	
	35/7.1		•
		·	in the fields searched
ocumentati	on searched other than minimum documentation to the ex	tent that such documents are included	in the fields scatched
	ata base consulted during the international search (name	of data base and, where practicable,	search terms used)
		• •	
Please See	Extra Sheet.		
	•		
c. DOC	UMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where appro	opriate, of the relevant passages	Relevant to claim No.
			1
X	WAGNER et al. A structural role for hormone in the thyroid hormone receptor. Nature. 14 December 1995, Vol. 378, pages		
	690-697, especially page 690 and figure	1 and 2 and Table 1.	2-30
A	690-697, especially page 690 and ligare		
		•	
			1
İ			
Fui	rther documents are listed in the continuation of Box C.	See patent family annex.	the state of priority
	Special categories of cited documents:	•T• later document published after the date and not in conflict with the a	DDITCSOOD DOT CIRE IN MIGGISTURE
A	document defining the general state of the art which is not considered to be of particular relevance	the principle or theory underlying	
	earlier document published on or after the international filing date	"X" document of particular relevance; considered novel or cannot be con	rideted to madiae mi macinga and
1	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other	when the document is taken alone "Y" document of particular relevance;	the claimed invention cannot be
1	special reason (as specified)	"Y" document of particular relevance; considered to involve an inven- combined with one or more other	
•0•	document referring to an oral disclosure, use, exhibition or other means	combined with one or more outer being obvious to a person skilled	in the art
P	document published prior to the international filing date but later than	•&• document member of the same pa	tent family
Data of t	the priority date elaimed he actual completion of the international search	Date of mailing of the international	search report
1		2 9 FEB 2000	
01 DECEMBER 1999			100
Name an	nd mailing address of the ISA/US	Authorized officer	XI B
Commis Box PC	ssioner of Patents and Trademarks	MICHAEL PAK	-// The
Washin	gton, D.C. 20231	Telephone No. (703) 308-1235	'/ "(
Facsimil	e No. (703) 305-3230	1 ciepnone 140. (103) 300 1233	<u></u>

Form PCT/ISA/210 (second sheet)(July 1992)*

INTERNATIONAL SEARCH REPORT

International application No. PCT/US99/06899

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)			
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:			
1. Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely:			
2. Claims Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:			
3. Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).			
Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)			
This International Searching Authority found multiple inventions in this international application, as follows:			
Please See Extra Sheet.			
1. X As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.			
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.			
3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:			
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:			
Remark on Protest			
No protest accompanied the payment of additional search fees.			

Form PCT/ISA/210 (continuation of first sheet(1))(July 1992)*

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